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(54) Title: MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

(57) Abstract

Three-dimensional crystal structure(s) of deacetoxycephalosporin C synthase (DAOCS) are described. The X-ray co-ordinates provide precise 3-dimensional information of amino acids within the structure of DAOCS. Some of these are in complexes with iron and/or substrates. Information from the structures is used to modify enzymes of the cephalosporin biosynthesis pathway including DAOCS, deacetylcephalosporin C synthase DAOC/DACS, such that they accept unnatural substrates (e.g. penicillins G, V) in order to improve the production of beta-lactam antibiotics. The structures may be used to predict the structures of other 2-oxoglutarate dependent enzymes, thereby allowing the design of inhibitors, and new catalysts for the production of e.g. oxidised amino acids/peptides. Specific modifications of amino acid residues are proposed and exemplified.

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MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

- Penicillin and cephalosporin antibiotics are produced either directly by fermentation or by modification of fermentation derived materials containing a beta-lactam ring. The biosynthetic pathway to the penicillins and cephalosporins has been extensively studied and reviewed (J. E. Baldwin and C. J. Schofield, in 'The Chemistry of β-lactams (Ed. M. I. Page), Chapter 1, Blackie, London 1992; Ingolia and Queener, Med. Res. Rev., 1989, 9, 245-264; Aharonowitz, Cohen and Martin, Ann. Rev. Microbiol., 1992, 46, 461-495; Schofield, Bycroft, Baldwin, Hadju, Roach, Current Opinion in Structural Biology, 1997, 7, 857-864) and includes the following steps (Figure 1):
- 1. Conversion of the tripeptide: <u>L</u>-δ-α-aminoadipoyl-<u>L</u>-cysteinyl-<u>D</u>-valine (ACV) to isopenicillin N in a step catalysed by isopenicillin N synthase (IPNS). This step is common to both penicillin and cephalosporin biosynthesis.
- In some organisms (e.g. Penicillium chrysogenum and Aspergillus nidulans) isopenicillin N is converted by exchange of its <u>L</u>-δ-α-aminoadipoyl side chain to penicillins with other side chains, which are normally more hydrophobic than the side chain of isopenicillin N. This conversion is catalysed by an amidohydrolase/ acyltransferase enzyme. Examples of penicillins produced by this biosynthetic process include penicillin G (which has a phenylacetyl side chain) and penicillin V (which has a phenoxyacetyl side chain). These hydrophobic penicillins may be commercially produced via fermentation under the appropriate conditions.
 - 3. In other organisms (e.g. *Streptomyces clavuligerus* and *Cephalosporium acremonium*) isopenicillin N is epimerised to penicillin N. This reaction is catalysed by an epimerase enzyme.

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- 4. In some organisms (e.g. S. clavuligerus and C. acremonium) penicillin N is converted to DAOC. This reaction is catalysed by deacetoxycephalosporin C synthase (DAOCS) in some organisms (e.g. Streptomyces clavuligerus) and by deacetoxy/deacety/cephalosporin C synthase (DAOC/DACS) in others (e.g. C. acremonium).
- 5. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) DAOC is converted to deacetylcephalosporin C (DAC). This reaction is catalysed by deacetylcephalosporin C synthase (DACS) in some organisms (e.g. *S. clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. *C. acremonium*).

Further biosynthetic steps to give other cephalosporin derivatives may also occur, e.g. in *C. acremonium* DAC may be converted to cephalosporin C and in *Streptomyces spp*. DAC may be converted to cephamycin C. The genes encoding for each of the enzymes catalysing steps 1-6 above have been identified and sequenced.

Fermented penicillins, cephalosporins and their biosynthetic intermediates are useful as antibiotics or as intermediates in the production of antibiotics. Penicillins with hydrophobic side chains may be used for the preparation of cephalosporins or intermediates used in the preparation of cephalosporins, e.g. penicillins (including penicillin G and penicillin V) may be used to prepare C-3 exomethylene cephams which may be used as intermediates in the preparation of the commercial antibiotics, e.g. Cefachlor.

The enzymes IPNS, DAOCS, DACS and DAOC/DACS are

members of an extended family of Fe(II) utilising oxidase and oxygenase enzymes. Most of this family (including DAOCS, DACS and DAOC/DACS) utilise a 2-oxo acid (normally 2-oxoglutarate) as a cosubstrate in addition to dioxygen and the 'prime' substrate (e.g. penicillin N in the case of DAOCS). Since IPNS, does not use 2-oxoglutarate, it has a substantially different mechanism to the 2-oxoglutarate dependent oxygenases, and this gives

This invention is based on the determination of the three

rise to a significantly different active site.

The Invention

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dimensional crystal structure of DAOCS and the information and developments which come from it. The X-ray co-ordinates provide very detailed 3-dimensional information on the relationships between amino acid residues in the structure of DAOCS and on the binding modes of the Fe-cofactor and the substrates to DAOCS. The structure allows the modification of DAOCS and related enzymes of penicillin and cephalosporin biosynthesis (including DACS and DAOC/DACS) in order to alter their substrate and product selectivities. Since the DAOCS structures are the first from the family of 2-oxoglutarate dependent dioxygenases they also allow for the design of new inhibitors of this family of enzymes. Previously partial overviews of the structures of IPNS complexed to manganese and IPNS complexed to iron and ACV were reported (Roach et al., Nature, 1995, 375, 700-704; Roach et al., Nature, 1997, 387, 827). The structures, as defined by their X-ray co-ordinates, of IPNS complexed to manganese and in complexes with iron, ACV and/or substrate analogues have been reported in Baldwin, Hajdu, Roach, Hensgens,

Procedures have been developed for the production of 7-aminodeacetoxycephaosporin C (7-ADCA) in which recombinant *P. chrysogenum* strains into which the DAOCS gene has been introduced are used for the production of cephalosporins. In particular if adipic acid is added to these recombinant strains adipoyl-6-APA is produced, which is converted by DAOCS into adipoyl-7-ADCA from which the adipoyl side chain can be removed (EPA-A-0532341, Shibata *et al.*, Bioorg. Med. Chem. Letts, 1996, 6, 1579-1584).

Clifton, GB 9621486.1- (Oxygenase Enzymes and Method).

The IPNS gene sequence (and therefore the amino acid

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sequence) is related but significantly different to those of DAOCS, DACS, DAOC/DACS. It is likely that gross elements of the fold (i.e. significant elements within the 3-dimensional structure) of these enzymes will be conserved but that the active site architecture will be very significantly different. Structural elements conserved are likely to include the betabarrel 'jelly roll' core and certain alpha-helices (including alpha helix-10, as defined in Roach et al., Nature, 1995, 375, 700-704). The degree of similarity is insufficient to define the precise structure of DAOCS, DACS, or DAOC/DACS from the IPNS structures. To date no models of DAOCS, DACS, or DAOC/DACS based on the IPNS structure have been reported. Nor have any detailed studies on substrate binding of these enzymes been reported. One report (WO 97/20053) claims the use of products resulting from modification of certain residues in DAOCS for the improved conversion of penicillin G to phenyl acetyl (G)-7-aminocephalosporanic acid.

The three-dimensional structure of DAOCS is defined by the X-ray co-ordinates set out below (Structure A).

Also set out below is a high resolution crystal structure of a complex of prokaryotic DAOCS from *S. clavuligerus* with Fe(II) and 2-oxoglutarate (Structure B).

In part the present invention relates to the use of the structures of DAOCS in order to make modifications to it or DACS or DAOC/DACS in order that the modified enzymes catalyse the conversion of unnatural penicillins (e.g. penicillin G and penicillin V) to cephalosporins more efficiently than the wild-type enzyme. Further aspects of the invention relate to the use of the DAOCS structure in order to produce unnatural products in micro-organisms. Such products include exomethylene cephalosporins, with or without alpha-aminoadipoyl or hydrophobic side chain (e.g. phenylacetyl or phenoxyacetyl). Thus one aspect of this invention refers to the use of the structure of DAOCS for modifying DAOCS

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(or the closely related enzymes DACS or DAOC/DACS) in order to:

- (i) permit the enzyme to accept (or accept more efficiently) unnatural penicillin substrates for the preparation of new or commercially valuable antibacterial materials.
- enable the modified enzyme to produce unnatural (e.g. exomethylene cephams) or optimise the production of minor products (e.g. 3-β-hydroxycephams) for use as antibacterials or as intermediates in the preparation of antibacterials or commercially valuable compounds.

In another aspect this invention provides modified enzymes that result from application of the aforementioned techniques. These are enzymes having significant (as defined below) sequence and thus structural similarity with DAOCS. Thus, structures of these enzymes may be predicted on the basis of the DAOCS structures. Preferably there will be sequence similarity/identity between most of the modified enzyme and a major part of DAOCS. Previous sequence comparisons (Roach et al., Nature, 1995, 375, 700), using pairwise comparisons of the sequences followed by single linkage cluster analysis show that IPNS, DAOCS, DACS and DAOC/DACS cluster with standard deviations scores of >5.0 (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Scores over 5.0 and preferably over 6.0 indicate that the sequence alignments will be correct within all or most of the protein secondary structural elements (Barton, Methods in Enzymol., 1990, 183, 403); thus they have significantly similar sequences and hence structures. Note there are other criteria which may be used to ascertain significant sequence similarity for example % identity or % similarity of amino acids possessing side chains with similar physicochemical properties (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Thus, on the basis of sequence comparisons it is possible to predict the structure of one enzyme (e.g. DACS or DAOC/DACS) from another closely related enzyme (e.g. DAOCS). Further, it is recognised that although two enzymes may have structures in which secondary structural elements are

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largely or wholly conserved, differences in the structures of the two enzymes may result from the side chains of the amino acids forming the secondary structural elements. The effect of these differences, which alter the substrate/product selectivities of the compared enzymes, is predictable once the three-dimensional structure of one of the enzymes is known.

In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Modifications of this kind will permit the expansion of penicillin V or penicillin G to the corresponding cephalosporins. To achieve this it is desirable to increase the kcat/Km for the mutant as compared to the wild type DAOCS. Kinetic results indicate that apparent kcat values for penicillin N and penicillin G are similar but that Km is much higher for penicillin G. Thus based on these analysis, a decrease in the binding constant of DAOCS for penicillin G should make it possible to increase kcat/Km for penicillin G.

The side chain binding pocket of DAOCS is made of residues from different parts of the peptide chain, so it is likely that more than one residue will have to be altered to make a better penicillin G/V expander. Nevertheless some residues are more important than others. Examination of the interactions between the last few C-terminal residues (Thr-308 to Ala-311) of one DAOCS molecule and the active site of another in the crystal structure, suggests a binding mode for the penicillin nucleus which

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is shown in Figure 2 of the accompanying drawings. The penam C-3 carboxylate group probably occupies an analogous position to that of Ala-311 from a symmetry related molecule in the active site, forming electrostatic interactions with Arg-162 and Arg-160. The side chain of Arg-160 may also form a hydrogen bonding interaction with the β -lactam carbonyl.

It needs to be borne in mind that protein specificity is generally controlled by more than one amino acid. To alter the specificity of a protein in a major way is likely to require more than one of the mutational changes suggested below, although each of the mutations will contribute. With this in mind, preferred residues to modify for the expansion of a penicillin are as follows:

- a) Arg-266. This residue binds with the α -aminoadipate side chain of the natural substrate and should be changed to a residue of more hydrophobic character, e.g. Phe, Ala, Val, Leu, Ile.
- b) Thr-72. This should be changed to a hydrophobic residue e.g. Val, Leu, Ile, Phe, Ala, to help bind the hydrophobic side chain of penicillin G. It should be effective in combination with other mutants.
- c) Arg-74 may be usefully changed to a neutral or hydrophobic residue (Phe, Tyr, Val, Leu, Ile, Ala). Modification of Arg-75 may be necessary in addition because it forms a hydrogen-bonding network with Arg-74.
 - d) Glu-156. This residue binds with the α -aminoadipate side chain. It should be changed to one of Ala, Val, Leu, Ile, Phe, Tyr, Trp, Asn, Gln, Ser.
- e) The side chains of Leu-158, Asn-301 and Tyr-302 form part of the binding pocket for the penicillin side chain and can be usefully modified to more hydrophobic character.
 - f) Asn-304. This residue binds the amide linking the side chain to the penam nucleus. Modification is effected to expand penicillins with shortened or no side chains (e.g. to Asp or Glu for 6-Apa).

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Note that other changes may be used to construct part or all of a side chain binding pocket via hydrogen bonding or other interactions.

The insertion or deletion of residues into the DAOCS sequence may also be of use in constructing a hydrophobic binding pocket for the penicillin side chain. Insertion of hydrophobic residues into the C-terminal region (residue 300-311 and in particular 301-303) may assist in the construction of a hydrophobic binding pocket for penicillin side chains.

In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Asn304, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Further discussion of this aspect may be found in Nature Volume 394, pages 805-809 published on 20 August 1998 and incorporated by reference herein.

Another aspect of the invention refers to the use of the structure of DAOCS in order to modify its active site (or that of a structurally related 2-oxoglutarate dependent dioxygenase) in order that the modified enzyme accepts non beta lactam substrates in order to produce oxidised compounds of value. Oxidised amino acids (e.g. 4-hydroxyprolines, hydroxylysines, hydroxyaspartic acids and others) are useful as synthetic intermediates in the production of valuable materials. Using the structure of DAOCS specific residues can be targeted for modification in order that the modified enzyme can be used to produce oxidised amino acids or peptides. The process may include modification of the following residues:

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Arg74, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304, Ile88, Arg162, Phe164, Met180, Thr190, Ile192, Pro241, Val245, Val262, Ile305, Arg306, Arg307.

Another aspect of the invention refers to the use of the DAOCS structure for the design of selective inhibitors of 2-oxoglutarate dependent dioxygenases. The 2-oxoglutarate dependent dioxygenase prolyl 4-hydroxylase has been the target of inhibition in order to provide a therapeutic treatment for fibrotic diseases (e.g. liver cirrhosis, arthritis). However, no inhibitors are in clinical use, probably because it is difficult to achieve selective inhibition of the target enzyme for inhibition over other enzymes (including 2-oxoglutarate dependent enzymes). The structure of

DAOCS provides a template for the design of inhibitors of 2-oxoglutarate dependent dioxygenases.

Set out below are two high resolution crystal structures for DAOCS from *S. clavuligerus*: the structure of the iron-free apoenzyme (Structure A) and the structure of the complex with Fe(II) and 2-oxoglutarate (Structure B). The results imply a mechanism by which the enzyme-Fe(II) complex reacts with 2-oxoglutarate and dioxygen to give the reactive ferryl species, a process common to many non-haem oxygenases. Other notable 2-oxoacid-dependent ferrous enzymes are prolyl hydroxylase, involved in collagen biosynthesis, gibberellin 3β-hydroxylase, a mutation of which influences stem length in plants, and clavaminic acid synthase, involved in the biosynthesis of the β-lactamase inhibitor, clavulanic acid. Within the family of 2-oxoacid-dependent enzymes, DAOCS belongs to a sub-family, the members of which show sequence similarity with IPNS and 1-aminocyclopropane-1-carboxylate oxidase (the ethylene forming enzyme), enzymes that do not use a 2-oxoacid in catalysis.

The iron-free form of DAOCS crystallises in space group R3

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as a crystallographic trimer. The main chain of the protein folds into a conserved jelly roll core with flanking helices.

Co-ordinates and structure factors have been deposited with the Protein Data Bank (entries 1rxg, and r1rxgsf for the Fe(II)-2-oxoglutarate complex).

LEGENDS TO FIGURES.

Figure 1: the biosynthetic pathway to the penicillins and cephalosporins.

Figure 2 is a view of the active site of DAOCS showing 2-oxoglutarate binding to the iron and proposed penicillin N binding. Interactions with the side chains of certain amino acid residues are indicated by arrows.

Structure A is a three-dimensional structure of DAOCS.

Structure B is a high resolution crystal structure for prokaryotic DAOCS from *S. clavuligerus* as a complex with Fe(II) and 2-oxoglutarate.

The peptide sequence of DAOCS (with the numbering used herein) is set out below:

	Met	Asp	Thr	Thr	Val	Pro	Thr	Phe	Ser	Leu	10
	Ala	Glu	Leu	Gln	Gln	Gly	Leu	His	Gln	Asp	20
	Glu	Phe	Arg	Arg	Cys	Leu	Arg	Asp	Lys	Gly	30
	Leu	Phe	Tyr	Leu	Thr	Asp	Cys	Gly	Leu	Thr	40
5	Asp	Thr	Glu	Leu	Lys	Ser	Ala	Lys	Asp	Leu	50
	Val	Ile	Asp	Phe	Phe	Glu	His	Gly	Ser	Glu	60
	Ala	Glu	Lys	Arg	Ala	Val	Thr	Ser	Pro	Val	70
	Pro	Thr	Met	Arg	Arg	Gly	Phe	Thr	Gly	Leu	80
	Glu	Ser	Glu	Ser	Thr	Ala	Gln	Ile	Thr	Asn	90
10	Thr	Gly	Ser	Tyr	Ser	Asp	Tyr	Ser	Met	Cňa	100
	Tyr	Ser	Met	Gly	Thr	Ala	Asp	Asn	Leu	Phe	110
	Pro	Ser	Gly	Asp	Phe	Gly	Arg	Ile	Trp	Thr	120
	Gln	Tyr	Phe	qaA	Arg	Gln	Tyr	Thr	Ala	Ser	130
	Arg	Ala	Val	Ala	Arg	Glu	Val	Leu	Arg	Ala	140
15	Thr	Gly	Thr	Glu	Pro	Asp	Gly	Gly	Val	Glu	150
	Ala	Phe	Leu	Asp	Cys	Glu	Pro	Leu	Leu	Arg	160
	Phe	Arg	Tyr	Phe	Pro	Gln	Val	Pro	Glu	His	170
	Arg	Ser	Ala	Glu	Glu	Gln	Pro	Leu	Arg	Met	180
	Ala	Pro	His	Tyr	Asp	Leu	Ser	Met	Val	Thr	190
20	Leu	Ile	Gln	Gln	Thr	Pro	Cys	Ala	Asn	Gly	200
	Phe	Val	Ser	Leu	Gln	Ala	Glu	Val	Gly	Gly	210
	Ala	Phe	Thr	qzA	Leu	Pro	Tyr	Arg	Pro	Asp	220
	Ala	Val	Leu	Val	Phe	Cys	Gly	Ala	Ile	Ala	230
	Thr	Leu	Val	Thr	Gly	Gly	Gln	Val	Lys	Ala	240
25	Pro	Arg	His	His	Val	Ala	Ala	Pro	Arg	Arg	250
	Asp	Gln	Ile	Ala	Gly	Ser	Ser	Arg	Thr	Ser	260
	Ser	Val	Phe	Phe	Leu	Arg	Pro	Asn	Ala	Asp	270
	Phe	Thr	Phe	Ser	Val	Pro	Leu	Ala	Arg	Glu	280
	Cys	Gly	Phe	Asp	Val	Ser	Leu	Asp	Gly	Glu	290
30	Thr	Ala	Thr	Phe	Gln	Asp	Trp	Ile	Gly	Gly	300
	Asn	Tyr	Val	Asn	Ile	Arg	Arg	Thr	Ser	Lys	310
	Ala										311

- 12 -

STRUCTURE A

CRYST1	106.400	106.40	0	71.100		00.00	00.00	
SCALE1	0.009	398	0.0054			90.00	90.00	120.00
SCALE2			0.00542	•	0.0000	00	0.00000	00
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SCALE3	0.0000	000	0.00000	00	0.01406	55	0.00000	00

- 13 -

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ANISOU
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ANISOU 5
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ATOM
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                                   12.015
ANISOU 6
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ATOM
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MOTA
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 ATOM
                                                         148
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23.322 42.276 1.000 27.66
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 ATOM 159
ANISOU 159
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                   GLN
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 ATOM
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                   GLN
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 ANISOU 161
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 ANISOU 164 N
                   ASP
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 ATOM
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ANISOU 165 CA ASP
ATOM 166 C ASP
ANISOU 166 C ASP
ATOM 167 O ASP
                         20
                         20
                              1869
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                                                3235
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20 1429 2884 3848 -311 225 2
 ANISOU 167 O ASP
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ATOM
         168 CB ASP
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ANISOU 168
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                                                        -16
ATOM
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                                                               207 881
         169
              CG ASP
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ANISOU 169
              CG ASP
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20 33.870 19.914 43.153 1.000 35.78
                         20 2355
                                                               1323 - 1915
ATOM
         170
              OD1 ASP
ANISOU 170
              OD1 ASP
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                         20 3152 5452 4992 -741 1508 -
20 35.508 20.433 44.467 1.000 45.22
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ATOM
         171
              OD2 ASP
ANISOU 171
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MOTA
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ANISOU 172
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21 1386 2342 3050 -307 -395 2
21 28.290 19.602 49.054 1.000 18.46
21 1671 2286 3057 -419 -351 1
21 30.415 22.058 49.563 1.000 20.10
21 1646 2821 3170 -514 -499 1
21 31.893 22.322 49.918 1.000 24.11
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ANISOU 174
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ATOM
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ANISOU 175
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                                                        -419 -351 1 1 6
ATOM
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ANISOU 176
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                  GLU
                                                        -514 -499 1 2 7
ATOM
        177
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                  GLU
                         21
                             31.893 22,322
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ANISOU 177
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ATOM
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ANISOU 179
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MOTA
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                                                        -2089 -1618 647
ATOM
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ANISOU 181
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ATOM
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ANISOU 182
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              CA
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ATOM
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ANISOU 183
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                   PHE
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- 19 -ATOM 184 0 PHE 22 25.867 18.574 46.995 1.000 15.87 ANISOU 184 0 PHE 22 1570 2118 2343 -249 -361 1 3 1 MOTA 185 CB PHE 26.305, 21.840 46.149 1.000 18.00 22 ANISOU 185 CB PHE 22 1747 2754 2337 70 -178 445 ATOM 186 CG PHE 22 24.802 21.729 45.930 1.000 16.38 ANISOU 186 CG PHE 22 1763 1748 2714 -90 -326 2 2 3 187 CD1 PHE 22 23.934 21.723 47.003 1.000 18.29 ANISOU 187 CD1 PHE 22 1812 2091 3045 -197 -88 576 ATOM 188 CD2 PHE 22 24.290 21.720 44.641 1.000 18.62 ANISOU 188 CD2 PHE 22 2106 2079 2890 -143 -623 3 9 4 ATOM 189 CE1 PHE 22 22.569 21.727 46.771 1.000 18.90 ANISOU 189 CE1 PHE 22 1826 2086 3271 -198 -133 3 0 2 ATOM 190 CE2 PHE 22 22.911 44.379 1.000 19.28 21.660 ANISOU 190 CE2 PHE 22 2189 3114 2023 -242 -754 - 144 ATOM 191 CZPHE 22 22.059 21.645 45.473 1.000 19.42 ANISOU 191 CZPHE 22 2048 1723 3607 90 - 483 - 376 ATOM 192 N ARG 23 27.580 18.971 45.583 1.000 17.88 ANISOU 192 N ARG 23 1647 2437 2709 -168 -218 3 1 7 ATOM 193 CA ARG 23 27.520 17.594° 45.079 1.000 19.18 ANISOU 193 CA ARG 23 1724 2539 3022 -166 36 158 ATOM 194 C 27.767 16.595 46.211 1.000 19.11 ARG 23 ANISOU 194 C ARG 23 1279 2461 3518 -173 -113 4 5 5 MOTA 195 0 ARG 23 27.107 15.547 46.229 1.000 18.82 ANISOU 195 0 ARG 23 1614 2156 3381 -33 181 -128 CB ARG ATOM 196 28.605 17.351 44.030 1.000 22.81 23 ANISOU 196 CB ARG 23 1934 4099 2633 -34 -105 - 354ATOM 197 CG ARG 23 28.248 17.790 42.617 1.000 24.82 ANISOU 197 CG ARG 23 2601 4078 2752 191 -122 - 204ATOM 198 CD29.376 17.272 41.685 1.000 29.71 ARG 23 ANISOU 198 CDARG 23 2503 5619 3168 -285 908 704 MOTA 199 ΝE ARG 23 30.479 18.206 41.800 1.000 30.96 ANISOU 199 ΝE ARG 23 2877 5034 3851 -43 286 297 ATOM 200 CZARG 23 30.549 19.360 41.148 1.000 29.49 ANISOU 200 CZARG 23 2612 5063 3529 -225 606 177 ATOM 201 NH1 ARG 23 29.536 19.665 40.328 1.000 29.26 ANISOU 201 NH1 ARG 23 3242 4951 2923 -960 331 ATOM 202 NH2 ARG 23 31.629 20.092 41.345 1.000 32.61 ANISOU 202 NH2 ARG 23 2320 5347 4722 -134 519 1 28.708 16.851 47.125 1.000 17.80 4722 -134 519 179 MOTA 203 N ARG 24 ANISOU 203 1262 2168 3332 183 38 9 0 28.930 15.899 48.222 1.000 18.85 N ARG 24 ATOM 204 CA ARG 24 ANISOU 204 CA ARG 1368 2509 3287 69 -162 10 9 27.701 15.811 49.114 1.000 17.51 24 69 -162 105 ATOM 205 C ARG 24 ANISOU 205° C ARG 24 1456 2015 3181 132 -177 2 4 3 ATOM 27.333 14.733 49.544 1.000 17.93 206 0 ARG 24 ANISOU 206 0 ARG 24 1851 1965 2997 -16 -402 2 5 3 30.203 16.321 48.991 1.000 19.88 1685 2700 3169 -398 -218 4 31.459 16.053 48.135 1.000 29.07 ATOM 207 CB ARG 24 ANISOU 207 CB ARG 24 3169 -398 -218 4 4 ATOM 208 CG ARG 24 ANISOU 208 CG ARG 1467 4625 24 4954 269 203 709 ATOM 209 CD32.700 16.206 49.016 1.000 41.84 ARG 24 ANISOU 209 CDARG 24 1745 7021 7130 -451 -494 - 922 ATOM 210 ΝE ARG 24 33.690 17.103 48.464 1.000 57.06 ANISOU 210 ΝE ARG 24 4362 9316 8003 -3326 -669 -1141 ATOM 211 CZARG 34.032 18.327 24 48.810 1.000 60.67 ANISOU 211 CZARG 5961 24 10369 6723 -4627 -1324 -1586 MOTA 212 NH1 ARG 33.430 18.980 24 49.799 1.000 49.70 ANISOU 212 NH1 ARG 24 7748 6565 4569 -951 -2185 2226 ATOM 213 NH2 ARG 24 34.997 18.971 48.159 1.000 54.12 ANISOU 213 NH2 ARG 24 8696 8490 3378 -3780 -2352 1607 ATOM 214 CYS 25 16.963 49.370 1.000 15.74 27.092

						PCT/GB98/03860
ANISOU 21		(S 25	1435	- 20 -		-
ATOM 21	.5 CA CY	S 25	25.884	1969 1 16.92	2574 1 50.22	
ANISOU 21 ATOM 21			1518	1954	2756	
ANISOU 21	6 C CY			16.06	8 49.54	-95 -317 -300 7 1.000 15.73
ATOM 21	7 0 0		1629 24.124	1699	2648	-114 -43266
ANISOU 21	7 0 CY		1453	15.262 1801		5 1.000 15.89
ATOM 21		S 25	25.367	18.362	2783	-88 -459 2 5 2
ANISOU 21 ATOM 21			1644	1779	2629	4 1.000 15.93
ANISOU 21			23.700	18.417	7 51.18	-49 -261 - 3 0 4 1.000 17.82
ATOM 22	0 N T.F.		1742 24.623	1825	3202	-122 -33 -55
ANISOU 22	O N LE		1449	16.308 1843	48.25 2504	0 1.000 15.25
ATOM 22: ANISOU 22:			23.560	15.590	230 <u>4</u>) 47 53.	-54 -263 -142 4 1.000 15.62
ATOM 22			1616	1739	2580	-86 -453 4 8
ANISOU 222	2 C LE		23.763 1697	14.085	47.62	1 1.000 15.18
ATOM 223	O LE	J 26	22.819	1764 13.345	2306	-113 -479 6
ANISOU 223 ATOM 224			1797	1725	2920	1.000 16.96 -234 -664 - 300
ANISOU 224	CB LET		23.526	16.068	46.066	-234 -664 -300 5 1.000 16.02
ATOM 225	CG T.FT		1811 23.057	1645	4633	-191 ~483 1 2 2
ANISOU 225 ATOM 226	(J 26	1762	17.510 1716		1.000 15.69
ATOM 226 ANISOU 226	CD1 LEU		23.252	17.880	2485 44 405	-6 -15 7 9 1.000 17.48
ATOM 227		J 26 J 26	1750	2360	2532	-17 -130465
ANISOU 227	CD2 LEU	26	21.584 1655	17.680 2188	46.290	1.000 17.11
ATOM 228 ANISOU 228	N ARG	27	25.027	13.648	266U	-29 -75 160
ATOM 229	N ARG		1870	1818	2871	1.000 17.26 155 -326 140
ANISOU 229	CA ARG		25.295 2108	12.205	47.372	1.000 18.75
ATOM 230 ANISOU 230	C ARG	27	25.240	1845 11.599	3170	270 -955 102
ANISOU 230 ATOM 231	C ARG		1667	1801	3351	1.000 17.95 159 -897 2 1 9
ANISOU 231	O ARG		24.777	10.454	48.913	1.000 20.99
ATOM 232	CB ARG		2158 26.641	1793 12.008	4026	-43 -360 1 6 8
ANISOU 232 ATOM 233	CB ARG	27	2815	2034	46.670 3264	
ANISOU 233	N ASP N ASP	28	25.827	12.293	49.723	622 -377 -129 1.000 16.71
ATOM 234	CA ASP	28 28	1487 26.034	2004	2856	178 -328 6 7
ANISOU 234 ATOM 235	CA ASP		1613	11.672 2095	51.026 2931	1.000 17.47
ATOM 235 ANISOU 235	C ASP	28	24.872	11.866	2931 51 990	107 -301 1.2 7 1.000 17.22
ATOM 236	C ASP O ASP		1414	2204	4853	223 -447 4 7 1
ANISOU 236	O ASP		24.816 1932	11.081	52.937	1.000 17.62
ATOM 237 ANISOU 237	CB ASP	28		2139 12.237	2624	150 -565 3 2 7
ATOM 238	CB ASP	28	1581	3894	2948	1.000 22.17 -272 -467 5 5 9
ANISOU 238	CG ASP	28 ; 28 ;	28.590 1596	11.906	50.941	1.000 24.72
ATOM 239	OD1 ASP	28	~ ~ -	3323 10.905	4472	236 -288 648
ANISOU 239 ATOM 240	OD1 ASP	28 2	2317	3071	50.199	1.000 27.56 808 -284 572
ANISOU 240	OD2 ASP OD2 ASP	28 2	29.573	12.617		808 -284 5 7 2 1.000 3 2 . 0 8
ATOM 241	N LYS		1584 24.098	4343	6261	-144 -470 4 1 6
ANISOU 241 ATOM 242	N LYS	29 1		12.942 1814	51.821	1.000 15.57
ATOM 242 ANISOU 242	CA LYS	29 2	23.048	13.305	52.778	5 -303 178 1.000 15.13
ATOM 243	C LYS	29 1 29 2	1584	1999	2165	-68 -500 - 96
ANISOU 243	C LYS	_		13.500 1352	52.118	1.000 14.56
ATOM 244 ANISOU 244	O LYS	29 2	0.688		2686	77 -452 106 1.000 16.21
	O LYS	29 1			2657	-177 -315 - 5
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- 21 -
ATOM
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ANISOU 245
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                                    1672
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 MOTA
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ANISOU 246
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                 LYS
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MOTA
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ANISOU 247
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        248
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ATOM
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ANISOU 248
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ATOM
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ANISOU 249
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MOTA
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ANISOU 253
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ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM	301 302 302 303 303 304 304 305	N CA C C C C C C C C C C C C C C C C C C	ASP ASP ASP ASP ASP ASP ASP ASP ASP	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	2287 18.240 2678 17.474 2104 17.929 2593 19.703 2666 20.588	1747 33.300 1722 32.711 1929 32.685 1749 33.561 2366 34.192	3040 49.884 3483 48.703 3586 47.540 3662 49.500 3406 50.551	-187 1.000 -632 1.000 198 1.000 -496 1.000 -876	-316 1 4 9 20.75 -508 3 7 4 20.05 -928 4 8 9 21.06 -756 1 3 1 22.21 -755 8 0 7
		CG	ASP	3 6	2537	1818	4402	-175	-833 - 208

- 23 -MOTA 306 OD1 ASP 36 20.061 34.886 51.457 1.000 26.16 ANISOU 306 OD1 ASP 3 6 2981 2100 4860 378 -777 - 381 307 OD2 ASP 36 21.824 33.982 50.528 1.000 24.87 ANISOU 307 OD2 ASP 36 2532 1994 4924 -49 -950 -628 MOTA 308 N CYS 37 15.282 32.196 48.971 1.000 20.25 ANISOU 308 N CYS 37 2135 1711 3849 118 -638 - 263 ATOM 309 CA CYS 37 15.463 31.587 47.902 1.000 20.28 ANISOU 309 CA CYS 37 2390 1478 3839 136 -799 -138 MOTA 310 C CYS 37 14.078 32.183 47.818 1.000 19.90 ANISOU 310 С CYS 37 2374 1724 3463 214 -711 - 74 ATOM 311 0 CYS 37 31.629 47.156 1.000 22.75 13.176 ANISOU 311 0 CYS 37 2569 1984 4091 -12 -1108 1 5 ATOM 312 СВ CYS 37 15.359 30.061 48.083 1.000 22.21 ANISOU 312 СB CYS 37 2739 4247 1454 194 -477 - 115 ATOM 313 SG CYS 37 14.500 29.595 49.596 1.000 22.84 ANISOU 313 SG. CYS 37 2854 1884 3942 -203 -922 1 4 1 MOTA 13.855 33.390 48.314 1.000 20.85 314 N GLY 38 ANISOU 314 N GLY 38 2353 1638 3933 -375 - 42 217 MOTA 315 CA GLY 12.570 34.044 48.194 1.000 23.42 38 ANISOU 315 CA GLY 38 2233 1874 4790 255 -292 1 6 5 MOTA 316 C GLY 11.534 33.619 49.217 1.000 23.29 38 ANISOU 316 С GLY 3.8 2577 2045 4228 113 -136 - 601 MOTA 317 0 GLY 34.091 49.129 1.000 25.58 38 10.400 ANISOU 317 0 GLY 38 2529 3424 3765 214 -96 -264 ATOM 318 N LEU 39 11.894 32.836 50.237 1.000 24.55 ANISOU 318 N LEU 39 2310 2980 4037 119 -46 -364 ATOM 319 CA LEU 39 10.938 32.331 51.195 1.000 24.44 39 2637 39 11 10 CA LEU ANISOU 319 2964 3684 -105 175 -946 MOTA 320 LEU 11.107 32.885 52.593 1.000 35.41 ANISOU 320 C 39 LEU 5341 4215 -796 165 -1435 3898 MOTA 321 0 LEU 39 11.784 32.313 53.441 1.000 43.41 ANISOU 321 0 LEU 39 7338 4986 4171 -2639 -1333 -303 ATOM 322 CB LEU 39 10.850 30.810 51.206 1.000 26.48 СВ ANISOU 322 LEU 39 4244 2940 2879 49 -70 - 261 ATOM 323 CG LEU 39 10.404 30.097 49.921 1.000 30.21 ANISOU 323 CG LEU 39 4834 2452. 4195 258 -1618 - 474ATOM 324 CD1 LEU 39 10.683 49.972 1.000 24.78 28.595 ANISOU 324 CD1 LEU 39 3351 2597 3468 424 -707 -118 ATOM 325 CD2 LEU 39 8.940 30.407 49.640 1.000 27.50 ANISOU 325 CD2 LEU 39 4828 2118 3503 860 -860 - 323ATOM 326 THR 40 10.365 33.957 52.882 1.000 45.58 ANISOU 326 THR 40 7392 5077 4849 -520 2852 -1993 ATOM 327 CATHR 40 10.610 34.661 54.136 1.000 32.50 ANISOU 327 CA THR 40 4224 3732 4393 999 961 - 558 ATOM 328 C THR 9.700 40 34.177 55.248 1.000 29.68 ANISOU 328 C THR 40 3175 4204 3898 -116 294 -1630 ATOM 329 0 THR 40 8.653 55.031 1.000 39.75 33.556 ANISOU 329 O THR 40 3930 5847 -1079 -301 -1653 5326 ATOM 330 CB THR 40 10.641 36.183 53.997 1.000 56.31 ANISOU 330 CB THR 40 10586 3758 7052 -1417 1006 - 992 ATOM 331 OG1 THR 40 11.545 36.606 52.946 1.000 68.39 ANISOU 331 OG1 THR 40 7379 3900 14707 -1978 3617 - 246 ATOM 332 CG2 THR 40 11.214 36.837 55.256 1.000 70.22 ANISOU 332 CG2 THR 40 8265 5228 13188 1389 -4422 -3241 ATOM 333 34.302 56.486 1.000 33.20 5223 3810 -203 307 -N ASP 41 10.191 ANISOU 333 N ASP 41 3580 -1779 MOTA 334 CA ASP 41 9.329 33.943 57.613 1.000 27.51 ANISOU 334 CA ASP 41 2705 3858 3891 91 -253 -1061 ATOM 335 C ASP 41 8.107 57.660 1.000 33.43 34.861 ANISOU 335 C ASP 41 3131 3064 6508 32 547 - 1307 ATOM 336 ASP 41 7.034 34.469 58.101 1.000 30.76

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- 25 -

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- 26 -ANISOU 397 O ASP 49 2863 3177 4257 -368 1004 -1544 398 CB ASP 49 -2.034 34.824 60.167 1.000 30.34 ANISOU 398 CB ASP 49 3695 3210 4623 -559 713 -2178 ATOM 399 CG ASP 49 -0.924 35.181 61.128 1.000 37.18 ANISOU 399 CG ASP 49 5259 4057 4810 -1109 -211 -2007 ATOM 400 OD1 ASP 49 -0.556 34.266 61.904 1.000 33.36 ANISOU 400 OD1 ASP 49 3717 4549 -737 888 -1727 4408 ATOM -0.525 36.375 61.087 1.000 48.45 401 OD2 ASP 49 ANISOU 401 OD2 ASP 49 7960 3575 6875 -927 -2887 -2409 MOTA 402 N LEU -3.788 33.402 50 58.059 1.000 24.46 Ν ANISOU 402 LEU 50 3114 2668 3513 374 200 -1298 CA LEU CA LEU ATOM 403 50 -5.123 33.344 57.471 1.000 22.92 ANISOU 403 LEU 50 2949 2145 3614 161 397 - 562 ATOM 404 С LEU -5.679 31.937 50 57.328 1.000 21.79 ANISOU 404 С LEU 50 3345 2197 2737 33 417 - 556 405 0 ATOM LEU -6.878 31.741 57.475 1.000 24.96 50 0 ANISOU 405 LEU 50 3463 2502 3517 - 276 766 - 1181 56.194 1.000 22.13 3517 ATOM 406 CB LEU 50 -5.254 34.137 ANISOU 406 CB LEU 50 3127 2016 3266 -103 524 -757 34.578 55.807 1.000 28.87 2016 ATOM 407 CGLEU 50 -6.661 ANISOU 407 CG LEU 50 3549 3538 3881 825 208 961 ATOM 408 CD1 LEU -7.389 35.082 57.049 1.000 52.72 50 ANISOU 408 CD1 LEU 50 4567 8556 6907 940 2929 -1936 ATOM 409 CD2 LEU 50 -6.644 35.642 54.723 1.000 41.07 ANISOU 409 CD2 LEU 50 6971 3395 5240 -1005 -2258 857 410 N ATOM VAL 51 -4.801 30.956 57.138 1.000 21.78 ANISOU 410 N VAL 51 3345 2052 2877 -160 216 -860 ATOM 411 CA VAL 51 2-5.293 29.580 57.118 1.000 19.40 ANISOU 411 CA VAL 51 2631 2056 2683 -12 173 - 303MOTA 412 С VAL -5.631 51 29.135 58.533 1.000 25.25 ANISOU 412 С VAL 51 4453 2656 2485 -753 587 - 955 ATOM 413 0 VAL 51 -6.652 28.454 58.725 1.000 25.07 ANISOU 413 0 VAL 51 4555 2176 2795 -484 1185 -827 ATOM 414 CB VAL 51 28.589 56.396 1.000 18.78 -4.377 ANISOU 414 CB VAL 51 2729 1786 2620 -72 171 - 3.13 ATOM 415 CG1 VAL 51 -3.152 28.238 57.231 1.000 20.42 ANISOU 415 CG1 VAL 51 3002 1841 2918 295 -13 - 480ATOM 416 CG2 VAL 51 -5.147 27.306 56.021 1.000 24.10 ANISOU 416 CG2 VAL 51 3112 2337 3708 -511 355 - 846 ATOM 417 -4.836 29.500 59.534 1.000 25.23 N ILE 52 ANISOU 417 N ILE 52 4514 2471 2603 388 76 -874 ATOM 418 CA ILE -5.205 29.114 60.921 1.000 24.38 52 ANISOU 418 CA ILE 52 3488 3010 2765 248 19 - 509 ATOM 419 C -6.498 29.771 61.355 1.000 24.20 ILE 52 ANISOU 419 C ILE 52 3026 2482 3687 -354 114 -648 ATOM 420 0 ILE 52 -7.328 29.182 62.071 1.000 27.73 ANISOU 420 O ILE 52 3735 2812 3989 -198 614 -334 421 CB ILE ATOM 52 -4.016 29.427 61.829 1.000 27.59 ANISOU 421 CB ILE 52 3321 4347 2815 590 0 - 785 ATOM 422 CG1 ILE 52 -2.853 28.439 61.510 1.000 31.45 ANISOU 422 CG1 ILE 52 3278 5248 3425 741 363 -1288 ATOM 423 CG2 ILE 52 -4.293 29.312 63.317 1.000 33.62 ANISOU 423 CG2 ILE 52 3827 6199 2750 881 150 -1454 ATOM 424 CD1 ILE 52 -1.930 28.351 62.710 1.000 36.22 ANISOU 424 CD1 ILE 52 3956 5082 4722 979 -601 -234 ATOM 425 ASP Ν 53 -6.771 30.992 60.913 1.000 24.56 ANISOU 425 Ν ASP 53 3479 2878 2974 165 609 -426 ATOM 426 CA ASP 53 -8.051 31.646 61.278 1.000 23.50 ANISOU 426 CA ASP 53 3242 2942 2745 -5 355 -677 MOTA 427 С ASP 53 -9.201 30.929 60.594 1.000 26.34 ANISOU 427 С ASP 53 3462 2986 3561 -435 612 -1064

- 27 -

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3958

CB

CB

ANISOU 488

GLU

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 MOTA
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NH1 ARG
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                    64
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            NH2 ARG
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 ATOM
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 AMISOU 527
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               VAL
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ANISOU 534 C
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ANISOU 535 O
                        1567 '2071
               VAL
                    66
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       536 CB
                                                    -106 - 317
ATOM
              VAL
                        -12.784 25.277 50.437 1.000 18.91
                    66
ANISOU 536 CB VAL
                    66
                        2175 1576
                                        3433
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ATOM
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           CG1 VAL
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ANISOU 537
           CG1 VAL
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ATOM
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           CG2 VAL
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ANISOU 538 CG2 VAL
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MOTA
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ANISOU 539
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ANISOU 540 CA THR
ATOM 541 C THR
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ANISOU 543
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               THR
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MOTA
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ANISOU 544
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ATOM
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ANISOU 545
           CG2 THR
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ATOM
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ANISOU 546
           N
               SER
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                                1720
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ANISOU 547
           CA SER
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                    68
ANISOU 548
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ATOM
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ANISOU 549
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                    68
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- 31 -ATOM 550 СВ SER 68 -11.958 17.303 47.257 1.000 17.84 ANISOU 550 CB SER 68 1459 2139 3182 -87 647 - 313 MOTA 551 OG SER 68 -10.998 18.259 46.904 1.000 17.21 ANISOU 551 OG SER 68 1659 1987 2893 -75 364 - 49 MOTA 552 PRO -14.929 16.284 47.054 1.000 15.89 N 69 ANISOU 552 PRO 69 M 1574 1661 2803 -201 -103 -280 ATOM 553 -15.877 15.182 CAPRO 69 47.339 1.000 16.42 ANISOU 553 CA PRO 69 1428 1903 2908 -251 -148 -218 ATOM 554 C PRO 69 -15.168 13.889 47.684 1.000 17.22 ANISOU 554 C PRO 69 1633 1578 3331 -199 266 -424 ATOM 555 0 PRO 69 -15.794 12.997 48.287 1.000 18.35 ANISOU 555 0 PRO 69 1815 1760 3399 -365 232 -376 ATOM 556 CB PRO 69 -16.712 15.057 46.060 1.000 16.75 ANISOU 556 CB PRO 69 1354 2279 2733 -360 155 -729 ATOM 557 CG PRO 69 -15.799 15.637 45.008 1.000 16.72 ANISOU 557 CG PRO 69 1553 2827 1971 -359 38 - 452 MOTA 558 CDPRO 69 -15.059 16.797 45.681 1.000 17.10 ANISOU 558 CD PRO 69 1918 1804 2776 -344 - 119 - 313ATOM 559 Ν VAL 70 -13.884 13.746 47.366 1.000 18.07 ANISOU 559 Ν VAL 70 1716 1764 3384 -89 292 - 215 ATOM 560 CAVAL 70 -13.100 12.594 47.824 1.000 17.34 ANISOU 560. CA VAL 70 1763 1851 2974 -20 260 - 196 ATOM 561 С VAL 70 -11.995 13.142 48.720 1.000 17.59 ANISOU 561 C VAL 70 2207 2788 1686 -180 159 -142 ATOM 562 0 VAL 70 -11.431 14.186 48.389 1.000 18.59 ANISOU 562 0 VAL 70 1794 1688 3581 -49 1 5 2 ATOM 563 CВ VAL 70 -12.429 11.757 46.724 1.000 18.10 ANISOU 563 CВ VAL 70 1922. 1756 3199 -353 560 -446 564 ATOM CG1 VAL 70 46.213 1.000 20.54 -13.441 10.754 ANISOU 564 CG1 VAL 70 1927 2611 3268 76 - 663 -369 MOTA 565 CG2 VAL 70 -11.760 12.608 45.642 1.000 17.65 ANISOU 565 CG2 VAL 70 2379 1806 2520 145 9 1 0 ATOM 566 Ν PRO 71 -11.697 12.466 49.815 1.000 16.21 ANISOU 566 Ν PRO 71 1653 1810 2695 -34 464 - 156 MOTA 567 CAPRO 71 -10.839 13.091 50.833 1.000 17.32 ANISOU 567 CAPRO 71 1795 1931 2854 -121 184 - 12 ATOM 568 С PRO 71 -9.356 12.804 50.590 1.000 17.67 ANISOU 568 С PRO 71 1865 1927 2921 46 -57 1 5 6 ATOM 569 0 PRO 71 -8.585 12.223 51.350 1.000 20.57 ANISOU 569 0 PRO 71 2218 2247 3350 424 28 4 7 4 ATOM 570 CB PRO 71 -11.362 12.458 52.117 1.000 19.76 71 ANISOU 570 CB PRO 2976 1862 2668 -347 479 - 304 71 ATOM 571 CG PRO -11.721 11.056 51.670 1.000 19.08 ANISOU 571 71 CG PRO 2838 1805 2608 -267 259 - 234 ATOM 572 CD PRO 71 -12.323 11.220 50.286 1.000 17.97 ANISOU 572 71 CDPRO 2314 1974 2538 -390 451 -167 ATOM 573 N THR 72 -8.894 13.338 49.446 1.000 17.15 ANISOU 573 N THR 72 1677 2231 -215 2610 -17 -165 ATOM 574 CATHR 72 -7.57313.012 48.935 1.000 16.83 ANISOU 574 CATHR 72 1721 1863 2810 -60 -134 -472 ATOM 575 C THR 72 -6.490 14.000 49.358 1.000 15.20 ANISOU 575 C THR 72 1791 1623 .2362 -304 163 - 73 MOTA 576 0 THR 72 -5.320 13.729 49.104 1.000 17.49 ANISOU 576 0 THR 72 1776 1961 2908 -61 -31 -225 MOTA 577 CВ THR 72 -7.53312.971 47.399 1.000 16.18 ANISOU 577 CВ THR 72 1552 1848 2748 -146 -86 -261 ATOM 578 OG1 THR 72 -8.091 14.238 47.005 1.000 17.81 ANISOU 578 OG1 THR 72 1856 1880 3031 -34 115 -191 MOTA 579 CG2 THR 72 -8.338 11.816 46.825 1.000 17.49 ANISOU 579 CG2 THR 72 1953 2087 2605 -550 181 -329 ATOM 580 MET 73 -6.877 15.098 49.987 1.000 17.78

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ATOM
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MOTA
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MOTA
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ATOM
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ATOM
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ANISOU 593
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ATOM
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MOTA
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ANISOU 595
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ATOM
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ANISOU 596
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               ARG
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ATOM
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ATOM
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ATOM
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ANISOU 599
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ATOM
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ANISOU 600
            CA ARG
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                                        2272
                                               236
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ATOM
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ANISOU 601
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ATOM
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ANISOU 608
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ATOM
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ANISOU 610
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ATOM	611	CA	\mathtt{GLY}	76	-8.858	22.532	49 637	1.000 16.67
ANISOU	611	CA	GLY	76	1650	2260	2425	-70 199 -612
MOTA	612	С	GLY	76	-8.602	22.002	51.036	
ANISOU	612	С	GLY	76	1584	2014	2602	
ATOM	613	O	GLY	76	-7.469	21.651		
ANISOU		Ö	GLY	76	1638	1998	2773	
ATOM	614	N	PHE	77	-9.643	22.025		
ANISOU		N	PHE	77	1597	2141	2675	1.000 16.88
ATOM	615	CA	PHE	77	-9.584	21.646		-7 283 -191
ANISOU		CA	PHE	77	1838	21.040	2656	1.000 17.61
ATOM	616	C	PHE	77	-9.776	20.154	53.512	109 328 -114
ANISOU		C	PHE	77	1855	2248	2600	
ATOM	617	0	PHE	77	-10.589	10 500		-68 243 -185 1.000 18.23
ANISOU		O	PHE	77	1844	2488	2594	
ATOM	618	CB	PHE	77	-10.698		53.998	
ANISOU		CB	PHE	77	1730	2515	2480	· · · ·
MOTA	619	CG	PHE	77	-10.877	22 081	55.473	162 65 - 344
ANISOU	619	CG	PHE	77	2405	2530	2515	
ATOM	620		PHE	77	-9.966	22.594	56.395	
ANISOU			PHE	77	2514	3523	2426	
ATOM	621		PHE	77	-11.917			431 -23 -527 1.000 21.31
ANISOU	621		PHE	77	3282	2070	2743	36 615 - 288
ATOM	622		PHE	77	-10.116	22 294		1.000 21.05
ANISOU	622		PHE	77	2719	2768	2510	
ATOM	623		PHE	77	-12.079	20 991		171 221 - 339 1.000 25.09
ANISOU	623		PHE	77	2967	4120	2447	-501 625 -826
MOTA	624	CZ	PHE	77	-11.175	21 523		1.000 23.79
ANISOU	624	CZ	PHE	77	2263	3681	3095	-1 376 - 756
ATOM	625	N	THR	78	-9.022	19.631		1.000 17.64
ANISOU		N	THR	78	1616	2161	2925	37 336 1
MOTA	626	CA	THR	78	-9.296	18.279		1.000 18.12
ANISOU	626	CA	THR	78	1926	2243	2717	-157 624 - 28
ATOM	627	С	THR	78	-9.291	18.316		1.000 18.66
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ATOM	628	0	THR	78	-8.335	18.821	57.095	
ANISOU	628	0	THR	78	2158	2883.	3098	-432 90 1 7 7
ATOM	629	CB	THR	78	-8.252	17.242		1.000 21.00
ANISOU	629	CB	THR	78	2973	2067	2939	113 428 -574
ATOM	630		THR	78	-8.027	17.392		1.000 21.18
ANISOU	630	OG1	THR	78	2544	2671	2833	160 317 - 773
ATOM	631		THR	78	-8.735	15.832		1.000 26.65
ANISOU	631	CG2	THR	78	3759	2227	4141	-275 853 -618
ATOM	632	N	${ t GLY}$	79	-10.311	17.804		1.000 20.36
ANISOU		N	GLY	79	2669	2379	2690	-670 630 -144
ATOM	633	CA	GLY	79	-10.344	17.679		1.000 25.96
ANISOU	633	CA	GLY	79	3871	3249	2745	-790 576 375
ATOM	634	С	\mathtt{GLY}	79	-10.029	16.238		1.000 39.70
ANISOU		С	GLY	79	6407	3542	5135	-1658 -1944 1511
ATOM	635	0	GLY	79	-10.623	15.303	58.491	1.000 31.02
ANISOU	635	0	\mathtt{GLY}	79	4327	3187	4272	-404 419 - 75
ATOM	636	N	LEU	80	-9.069	16.055	59.936	1.000 36.07
ANISOU		N	LEU	80	4380	4536	4788	1381 -564 -835
ATOM	637	C.A.	LEU	80	-8.634	14.713		1.000 32.52
ANISOU	637	CA	LEU	80	3640	4083	4632	611 -502 -898
ATOM	638	C	LEU	8 0	-9.131	14.311		1.000 39.82
ANISOU	638	C	LEU	80	5051	4652	5428	-128 418 -538
ATOM	639	0	LEU	80	-9.998	14.963		1.000 37.05
ANISOU	639	0	LEU	80	5057	3807	5213	-292 666 8 7
ATOM	640	CB	LEU	0 8	-7.122	14.580		1.000 38.36
ANISOU		CB	LEU	8 0	3821	5456	5299	1568 -33 -1406
ATOM	641	CG	LEU	8 0	-6.488	14.753		1.000 38.27

- 34 -CG LEU 80 3714 ANISOU 641 CG LEU 80 3714 5900 4926 725 -288 -1 5900 4926 725 -288 - 2588 642 CD1 LEU 80 2579 8505 6170 -1092 -76 3 CD2 LEU 80 -7.170 13.856 57.854 1.000 40.75 CD1 LEU 80 2579 ANISOU 642 6170 -1092 -76 3 7 ATOM 643 ANISOU 643 CD2 LEU 80 4296 5601 5587 -6.459 17.442 63.930 1.000 36.72 -1965 - 1793ATOM 644 N SER 98 ANISOU 644 Ν SER 98 3404 6429 4118 -2114 -698 1 -5.629 17.877 62.824 1.000 39.59 ATOM 645 CA SER ANISOU 645 CA SER ATOM 646 C SER ANISOU 646 C SER ATOM 647 O SER 4118 -2114 -698 1948 98 6031 5376 3635 -449 383 2 -6.402 18.372 61.610 1.000 29.89 98 6031 3635 -449 383 2177 98 98 3806 3509 4040 141 640 1204 -7.474 17.856 61.304 1.000 38.27 98 ANISOU 647 0 98 4936 4300 SER 5303 -1107 395 885 MOTA 648 C3 -4.694 16.739 62.358 1.000 44.06 SER 98 ANISOU 648 CB SER 98 3175 7425 6141 633 -753 2704 ATOM 649 OG -3.672 17.368 61.583 1.000 46.84 98 SER ANISOU 649 OG SER 98 3497 6*3*02 7797 95 -408 2418 ATOM 650 N -5.829 19.317 60.869 1.000 28.56 MET 99 ANISOU 650 N MET 99 5029 3458 2365 -1080 -550 5 4 6 ATOM 651 CA MET 99 -6.426 19.941 59.700 1.000 21.44 ANISOU 651 CA MET ATOM 652 C MET 99 2284 3549 2315 -182 157 132 -5.376 20.229 58.624 1.000 19.16 99 ANISOU 652 C ATOM 653 O ANISOU 653 O MET 99 2306 2592 2382 -433 60 1 3 7 -4.232 20.575 58.930 1.000 23.34 MET 99 MET 99 2489 3920 2460 -773 225 -4 99 -7.164 21.209 60.105 1.000 25.20 99 -773 225 -410 ATOM 654 CB MET ANISOU 654 CB MET 99 3172 99 3172 3375 3028 -572 661 -547 99 3-8.481 20.965 60.872 1.000 25.85 CG CG SD SD ATOM 655 MET ANISOU 655 MET 99 3172 3862 2787 -275 739 - 782 ATOM 656 MET 99 -9.251 22.517 61.389 1.000 32.21 99 4405 ANISOU 656 99 4405 MET 3750 ATOM 657 CE ANISOU 657 CE 4083 -133 1580 - 568 99 -8.884 22.461 63.145 1.000 76.12 MET MET 99 14782 11538 2603 -3321 3478 - 3241 658 N ATOM 100 -5.778 20.094 57.361 1.000 18.85 CYS ANISOU 658 N CYS 100 2434 2443 2285 -160 93 1 9 4 ATOM 659 CA CYS 100 -4.868 20.333 56.234 1.000 18.55 ANISOU 659 CA CYS 100 2251 2380 2418 92 127 2 3 6 660 C MOTA CYS 100 -5.496 21.312 55.228 1.000 16.26 ANISOU 660 C CYS ATOM 661 0 CYS ANISOU 661 O CYS 100 1741 2395 2586 -69 154 -104 100 -4.604 18.982 55.545 1.000 18.46 ATOM 662 CB CYS 100 2822 2081 2111 98 118 5 1 1 100 -3.243 18.974 54.329 1.000 22.76 100 2622 2968 3058 307 391 1 101 -4.697 22.069 54.498 1.000 17.49 ANISOU 662 CB CYS ATOM 663 SG CYS ANISOU 663 SG CYS ATOM 664 N TYR ANISOU 664 N TYR 101 1839 CA TYR 101 1839 2473 2332 46 291 2 2 4 CA TYR 101 -5.117 22.874 53.373 1.000 15.38 2332 46 291 2 2 4 ATOM 665 ANISOU 665 CA TYR 101 1946 1939 TYR 101 1946 1939 1960 -50 90 -20 TYR 101 -4.102 22.594 52.245 1.000 13.65 1960 -50 90 - 262 ATOM 666 С ANISOU 666 C TYR 101 1676 1543 1967 -2 -123 -151 ANISOU 667 O TYR 101 -2.896 22.629 52.475 1.000 15.95 ANISOU 667 O TYR 101 1611 2231 2217 43 233 101 1611 2231 2217 -43 -232 -212 668 CB TYR 101 -5.122 24.382 53.739 1.000 19.02 ATOM ANISOU 668 CB TYR 101 2816 2082 2328 234 48 - 519 101 -5.617 25.109 52.498 1.000 17.85 ATOM 669 CG TYR ANISOU 669 CG TYR 101 2084 1895 2804 18 -26 -231 670 CD1 TYR 101 -6.964 25.134 52.171 1.000 18.25 ANISOU 670 CD1 TYR 101 2042 1596 3298 29 28 - 496 ATOM 671 CD2 TYR 101 -4.730 25.778 51.658 1.000 17.77 ANISOU 671 CD2 TYR 101 2037 1611 3106 -46 -125 - 1 2 7

- 35 -MOTA 672 CE1 TYR 101 -7.406 25.796 51.036 1.000 19.63 ANISOU 672 CE1 TYR 101 1977 1776 3704 88 -241 -221 26.386 50.478 1.000 20.46 ATOM 673 CE2 TYR 101 -5.147 ANISOU 673 CE2 TYR 101 2060 2608 3108 239 40 182 ATOM 674 101 -6.504 CZ TYR 26.392 50.166 1.000 20.29 ANISOU 674 CZTYR101 2187 2397 3127 -73 -353 - 260 MOTA 675 101 -6.932 26.995 OH TYR 49.000 1.000 23.34 ANISOU 675 OH TYR 101 2790 2555 3523 -3 -641 5 2 102 -4.648 22.210 51.097 1.000 14.60 MOTA 676 N SER ANISOU 676 N SER 102 1618 1890 2041 -61 -109 - 477 102 -3.797 21.792 49.980 1.000 14.52 ATOM 677 CA SER ANISOU 677 CA SER 102 1684 1802 2030 -108 62 -276 102 -4.011 22.670 48.747 1.000 14.99 ATOM 678 С SER ANISOU 678 С SER 102 1545 1790 2361 -296 -41 2 1 102 -5.167 23.105 48.477 1.000 16.73 ATOM 679 0 SER ANISOU 679 0 SER 102 1589 2342 2425 2 128 - 3 MOTA 680 CB SER 102 -4.163 20.340 49.593 1.000 13.82 ANISOU 680 CВ SER 102 1692 1548 2013 174 9 -138 MOTA 681 102 -3.996 19.476 50.720 1.000 16.06 0G SER ANISOU 681 OG SER 102 1886 2066 97 -121 6 3 2153 ATOM 682 Ν MET 103 -2.978 22.775 47.920 1.000 14.47 ANISOU 682 N MET 103 1568 1724 2206 51 -59 1 5 2 CA MET ATOM 683 103 -3.102 23.552 46.687 1.000 16.58 ANISOU 683 MET $C^{\mathcal{F}}$ 103 2194 1933 2173 331 -74 253 MOTA 684 С MET 103 -2.150 23.013 45.608 1.000 14.41 ANISOU 684 С MET 103 1598 1793 2083 -202 -210 6 3 ATOM 685 0 MET 103 -1.15722.347 45.920 1.000 16.24 ANISOU 685 0 103 1527 2384 103 -2.716 25.004 MET 2259 -61 -23 468 MOTA 686 CB MET 46.835 1.000 28.78 ANISOU 686 CB MET 103 6537 1318 3081 859 -207 3 6 6 ATOM 687 CG MET 103 -3.258 25.986 47.801 1.000 22.60 ANISOU 687 CG MET 103 2531 2157 3900 -161 -57 -291 ATOM 103 -2.338 27.505 688 SD \mathtt{MET} 47.506 1.000 20.60 ANISOU 688 SD MET 103 2499 1927 3400 -4 -164 -226 MOTA 689 CE MET 103 -2.587 27.945 45.804 1.000 21.63 ANISOU 689 CE \mathtt{MET} 103 2319 2601 3300 308 209 - 236 ATOM 690 N 104 -2.439 23.430 GLY 44.378 1.000 15.44 ANISOU 690 N GLY 104 1468 2228 2169 -68 -120 1 6 4 ATOM 691 CAGLY 104 -1.511 23.199 43.276 1.000 16.13 ANISOU 691 CA GLY 104 1688 2202 2241 42 65 4 6 9 MOTA 692 C GLY 104 -1.583 24.355 42.294 1.000 15.76 ANISOU 692 C GLY 104 1706 1997 2286 -32 -194 3 8 8 MOTA 693 0 GLY 104 -1.987 25.478 42.653 1.000 19.06 ANISOU 693 0 GLY 104 1953 2032 3256 -71 144 MOTA 694 N THR 105 -1.151 24.092 41.054 1.000 16.73 ANISOU 694 N THR 105 1685 2385 2287 -375 -55 515 ATOM 695 CATHR 105 -1.115 25.205 40.094 1.000 17.06 ANISOU 695 105 1725 CA THR 2390 2369 -231 -148 5 7 7 ATOM 696 105 -2.513 25.631 С THR 39.635 1.000 19.55 ANISOU 696 С THR 105 1768 1817 3842 -160 -346 5 2 5 ATOM 697 0 105 -2.680 26.703 39.059 1.000 22.41 THR ANISOU 697 0 THR 105 2262 2116 4136 -119 -520 8 4 2 ATOM 698 CВ 105 -0.301 24.857 THR 38.840 1.000 17.57 ANISOU 698 CВ THR 105 1759 2877 2038 -394 -343 3 7 7 MOTA 699 OG1 THR 105 -0.865 23.675 38.217 1.000 18.66 OG1 THR ANISOU 699 105 2035 2449 2607 -140 -458 4 1 6 CG2 THR 700 105 1.155 24.590 39.178 1.000 18.95 ANISOU 700 105 1748 2853 CG2 THR 2601 -105 -248 2 9 6 701 106 -3.507 24.751 106 1596 2293 Ν ALA 39.741 1.000 16.52 ANISOU 701 N ALA2389 -180 -1 2 9 8 ATOM 702 CA ALA 106 -4.846 25.035 39.218 1.000 16.59

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- 36 -
  ANISOU 702 CA ALA 106 1692
                                           1952
                                                      2660
                                                            -214 -209 2 4 3
  ATOM
                     ALA 106 -5.848 24.142 39.923 1.000 17.52
           703
                С
 ANISOU 703 C
                     ALA 106 1651 1821 3186 26 -66 5 5 5
ALA 106 -5.479 23.323 40.805 1.000 17.88
 ATOM
           704 0
 ANISOU 704 O
                      ALA
                           106 2038
                                           2087
                                                      2668
                                                              59 -51 3 8 8
          705 CB ALA
 ATOM
                           106 -4.862 24.838 37.713 1.000 20.31
 ANISOU 705 CB ALA
                            106 2331
                                          2764
                                                              -197 -403 4 4 0
                                                     2620
          706 N
 ATOM
                            107 -7.149 24.329 39.717 1.000 18.00
                      ASP
 ANISOU 706 N
                     ASP
                            107 1576
                                          2208
                                                     3057 -77 -120 4 9
                            107 -8.217 23.535 40.344 1.000 17.46
 ATOM 707
               CA ASP
 ANISOU 707 CA ASP
                            107 1563 2191 2881 -83 -472 3
107 -8.173 23.753 41.859 1.000 17.74
                                                     2881 -83 -472 3 6 3
 ATOM 708 C
                     ASP
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107 -8.458 22.854 42.650 1.000 18.95
 ANISOU 708 C
                     ASP
                                                     2869 447 -269 3 6 2
 ATOM 709 O ASP
 ANISOU 709 C ASP
                           107 1994 2230 2974 167 -133 4 0 2
107 -8.089 22.044 39.990 1.000 19.62
 ATOM 710 CB ASP
ANISOU 710 CB ASP
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107 -8.370 21.842 38.508 1.000 20.81
                                                     2942 -394 -727 1 7 3
 ATOM 711 CG ASP
ANISOU 711 CG ASP
ANISOU 711 CG ASP

ATOM 712 OD1 ASP

ANISOU 712 OD1 ASP

ATOM 713 OD2 ASP

ANISOU 713 OD2 ASP

ATOM 714 N ASN

ANISOU 714 N ASN

ATOM 715 CA ASN

ANISOU 715 CA ASN

ANISOU 716 C ASN

ANISOU 716 C ASN

ANISOU 717 O ASN

ANISOU 717 O ASN
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                           107 1952 3093 2862 -138 -532 -
107 -9.369 22.369 37.976 1.000 25.84
                                                             -138 -532 - 14
                           107 2524
                                           3967
                                                     3327
                           107 -7.544 21.168 37.844 1.000 25.86
                                                                     -1149 - 240
                           107 3314
                                          2989
                                                     3523
                           108 -7.893 24.962 42.298 1.000 18.18
                                                             391
                                                                     -91 -89
                           108 2049 2075
                                                     2786
                           108 -7.831 25.263 43.740 1.000 17.10
                                                             509
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                           108 1804 1977
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                           108 -9.158 25.716 44.314 1.000 17.11
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                           108 -10.103 26.086 43.604 1.000 20.72
108 2066 2377 3430 759 -248 2
108 -6.799 26.379 43.969 1.000 19.90
ANISOU 717 O ASN
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ATOM
         718 CB ASN
                          108 1770 2308 3483 186 298 -
108 -5.400 25.862 43.717 1.000 17.24
ANISOU 718 CB ASN
                                                                     298 - 171
ATOM
         719
               CG ASN
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108 -4.986 24.850 44.277 1.000 17.42
ANISOU 719
               CG ASN
ATOM
         720
               OD1 ASN
               OD1 ASN 108 2003 1984 2631 109 11 -6
ND2 ASN 108 -4.644 26.487 42.834 1.000 18.41
ANISOU 720
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ATOM
         721
ANISOU 721 ND2 ASN
ATOM 722 N LEU
ANISOU 722 N LEU
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109 -9.308 25.509 45.607 1.000 18.09
              ND2 ASN
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ANISOU 722 N LEU
ANISOU 722 N LEU
ATOM 723 CA LEU
ANISOU 723 CA LEU
ATOM 724 C LEU
ANISOU 724 C LEU
ANISOU 725 O LEU
ANISOU 725 O LEU
ANISOU 725 C LEU
                          109 1795 2294 2786 349 344 1
109 -10.532 25.803 46.369 1.000 19.11
109 1763 2200 3296 14 476 - 598
109 -10.169 26.790 47.457 1.000 17.40
                           109 1682 1937 2990 251 129 -207
109 -9.443 26.423 48.395 1.000 21.18
                           109 2443 1922 3684 174 -520 2
109 -11.100 24.504 46.940 1.000 17.10
                           109 2443
         726 CB LEU
ATOM
ANISOU 726
               CB LEU
                           109 1888
                           109 1888 2142 2469 199 426 -630
109 -11.520 23.425 45.944 1.000 18.07
ATOM
         727
               CG LEU
ANISOU 727
               CG LEU
                           109 2515 1943
                                                   2409 190
                                                                     -198 - 363
ATOM
         728
               CD1 LEU
                           109 -11.895 22.124 46.654 1.000 20.06
ANISOU 728
               CD1 LEU
                           109 2842 2406
                                                   2375 -331 -175 - 200
ATOM
               CD2 LEU
                           109 -12.630 23.908 45.035 1.000 25.24
        729
ANISOU 729
               CD2 LEU
                           109 3481 2892 3217 306
                                                                  -992 -111
ATOM
        730 N
                           110 -10.609 28.036 47.313 1.000 17.25
                    PHE
ANISOU 730 N
                    PHE
                           110 1584 1926
                                                   3045 272 184 -132
ATOM
        731 CA PHE
                           110 -10.235 29.071 48.277 1.000 18.20
ANISOU 731 CA PHE
                           110 1751 1816
                                                   3346 169 221 -160
       732 C PHE
                          110 -11.409 29.567 49.106 1.000 19.93
ANISOU 732
                    PHE
                          110 2077
                                         1609 3886 71 650 - 335
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- 37 -MOTA 733 0 PHE 110 -12.433 29.948 48.494 1.000 24.64 ANISOU 733 0 PHE 110 2051 2461 CB PHE 4851 612 328 - 779 MOTA 734 110 -9.607 30.243 47.520 1.000 19.92 ANISOU 734 110 2367 1876 3324 224 619 - 93735 ATOM CG PHE 110 -8.380 29.986 46.688 1.000 19.47 ANISOU 735 CG PHE 110 2009 2209 3179 -321 327 -791 736 CD1 PHE MOTA 110 -7.177 29.680 47.287 1.000 20.59 ANISOU 736 CD1 PHE 110 2071 2080 3674 -274 236 -331 ATOM 737 CD2 PHE 30.035 45.299 1.000 20.19 110 -8.437 ANISOU 737 CD2 PHE 110 2557 1914 3200 112 543 - 289MOTA 738 CE1 PHE 110 -6.034 29.454 46.559 1.000 21.06 ANISOU 738 CE1 PHE 110 2020 2309 3673 -386 165 -622 ATOM 739 CE2 PHE 110 -7.277 29.811 44.547 1.000 20.77 ANISOU 739 CE2 PHE 110 2495 2138 3257 197 504 - 398 740 CZPHE 29.518 45.175 1.000 22.42 110 -6.081 ANISOU 740 CZPHE 110 2747 2092 3678 531 339 - 357 741 Ν PRO 111 -11.238 29.718 50.416 1.000 22.11 ANISOU 741 Ν PRO 111 2250 2153 3996 111 -12.287 30.389 51.195 1.000 28.23 -72 871 - 620 ATOM 742 CAPRO ANISOU 742 CA PRO 111 3895 2210 4621 698 1514 - 671 ATOM 743 111 -12.333 31.866 50.784 1.000 30.57 PRO ANISOU 743 C PRO 111 4528 2026 5061 410 410 -1041 ATOM 744 0 PRO 111 -11.390 32.340 50.115 1.000 31.71 ANISOU 744 O PRO 111 4040 2236 5774 -179 -597 - 12ATOM 745 CB PRO 111 -11.799 30.250 52.627 1.000 33.20 ANISOU 745 CВ PRO 111 5609 2702 4303 671 1671 - 790 ATOM 746 CG PRO 111 -10.646 29.326 52.647 1.000 26.04 ANISOU 746 CGPRO 111 2742 3316 3835 -931 1324 - 192 ATOM 747 CD 1112-10.161 29.149 51.230 1.000 22.15 PRO ANISOU 747 CDPRO 111 2587 2307 3522 -471 541 - 623 ATOM 748 N SER 112 -13.337 32.641 51.150 1.000 42.13 ANISOU 748 N SER 112 7176 2716 6115 2074 1731 - 526 MOTA 749 CA112 -13.368 34.026 50.672 1.000 44.05 SER ANISOU 749 CA 112 6799 2255 SER 7684 1107 -485 -826 750 C ATOM SER 112 -13.262 34.157 49.149 1.000 68.28 ANISOU 750 C SER 112 13632 4498. 7812 -1855 -2077 1301 MOTA 751 0 112 -12.347 34.825 48.646 1.000 95.18 SER ANISOU 751 0 112 15991 11425 SER 8747 -4337 -70 1985 752 CB SER 112 -12.493 35.069 51.349 1.000 39.31 ANISOU 752 CB SER 112 2247 4535 8153 580 1662 - 1437 753 ATOM OG 112 -11.474 34.624 52.213 1.000 37.49 SER ANISOU 753 OG SER 747 -1152 ATOM 754 N ASP 114 3476 2118 8237 1254 403 1 114 -8.205 37.586 50.600 1.000 30.79 ANISOU 754 N ASP 1254 403 1484 MOTA 755 CA ASP ANISOU 755 CA ASP 114 3503 2856 5340 1229 1240 9 9 6 114 -7.242 36.402 50.648 1.000 26.16 MOTA 756 C ASP ANISOU 756 C ASP 114 2581 2404 4955 601 1114 8 0 4 MOTA 757 O 114 -6.031 ASP 36.458 50.338 1.000 25.45 ANISOU 757 O 114 2302 ASP 4866 -43 602 131 2503 ATOM 758 CB ASP 114 -8.595 37.874 52.075 1.000 43.68 ANISOU 758 CB ASP 114 7509 2783 6304 1157 2727 - 210 38.386 52.835 1.000 46.96 2783 ATOM 759 CG ASP 114 -7.391 ANISOU 759 114 9259 CG ASP 3225 5359 2517 519 107 ATOM 760 OD1 ASP 114 -6.487 38.959 52.189 1.000 83.49 ANISOU 760 OD1 ASP 114 13724 9866 8132 -6354 650 -3056 761 114 -7.370 38.262 OD2 ASP 54.071 1.000113.59 ANISOU 761 OD2 ASP 114 27880 10550 4730 -6984 -159 -2575 ATOM 762 115 -7.831 35.323 N PHE 51.153 1.000 22.32 ANISOU 762 Ν PHE 115 2620 2062 3799 204 954 - 114 ATOM 763 CAPHE 115 -7.115 34.026 51.183 1.000 22.69

- 38 -ANISOU 763 CA PHE 115 2765 1909 3947 118 1093 - 187 ATOM 764 С PHE 115 -6.502 33.754 49.816 1.000 21.49 ANISOU 764 С PHE 115 2146 2316 3702 305 559 - 255 ATOM 765 0 PHE 115 -5.328 33.362 49.758 1.000 20.51 ANISOU 765 0 PHE 115 2153 2011 3627 323 488 -158 CB PHE ATOM 766 115 -8.096 32.928 51.638 1.000 20.76 ANISOU 766 PHE CB 115 2369 1946 3574 -3 563 -473 767 CGPHE 115 -7.496 31.590 51.998 1.000 20.23 ANISOU 767 CG PHE 115 2369 3463 -155 629 -377 51.041 1.000 20.35 1854 ATOM 768 CD1 PHE 115 -6.915 30.756 ANISOU 768 CD1 PHE 115 2572 3372 -195 112 -756 53.309 1.000 21.11 1786 ATOM CD2 PHE 769 115 -7.474 31.152 ANISOU 769 CD2 PHE 115 2802 1932 3287 -113 17 -689 115 -6.351 29.538 51.325 1.000 21.09 ATOM CE1 PHE 770 ANISOU 770 .CE1 PHE 115 2502 1728 3784 -295 471 -538 ATOM 771 115 -6.938 29.901 CE2 PHE 53.623 1.000 27.40 ANISOU 771 CE2 PHE 115 5012 1955 3445 444 43 - 572 ATOM 115 -6.332 29.110 772 CZ PHE 52.655 1.000 24.92 ANISOU 772 CZPHE 115 3356 1889 4222 50 1519 221 ATOM 773 N GLU 116 -7.301 33.768 48.757 1.000 21.64 ANISOU 773 N GLU 116 2396 1835 3990 338 261 - 13 ATOM 774 CA GLU 116 -6.750 33.424 47.444 1.000 20.90 ANISOU 774 CAGLU 116 2235 1965 3742 224 74 1 1 6 ATOM 775 С GLU 116 -5.550 34.262 47.054 1.000 20.32 ANISOU 775 C GLU 116 1978 1899 3845 439 -108 4 4 8 ATOM 776 0 116 -4.544 33.679 46.604 1.000 20.18 GLU ANISOU 776 O 116 2209 GLU 2147 3312 424 73 1 3 9 ATOM 777 CB 116 -7.851 33.561 46.385 1.000 24.22 GLU ANISOU 777 CB GLU 116 2425 2638 4139 -467 -237 5 1 9 ATOM 778 CG 116 -7.339 33.331 44.980 1.000 23.27 GLU ANISOU 778 CG GLU 116 2425 2465 3952 -7 -494 ATOM 779 CD 116 -8.401 33.273 43.910 1.000 25.02 116 2695 2703 4107 -510 -739 1 116 -9.617 33.306 44.207 1.000 34.83 GLU ANISOU 779 CD GLU -510 -739 1509 ATOM 780 OE1 GLU ANISOU 7.80 OE1 GLU 116 2466 4606 -203 -928 1566 6161 MOTA 781 OE2 GLU 116 -8.001 33.030 42.763 1.000 40.92 ANISOU 781 OE2 GLU 116 4389 7172 3988 -24 -968 6 9 3 ATOM 782 N 117 -5.549 ARG 35.571 47.300 1.000 20.60 ANISOU 782 N ARG 117 2299 1811 3718 382 -10 469 ATOM 783 CA ARG 117 - 4.37436.374 46.866 1.000 22.65 ANISOU 783 CA ARG C ARG 117 2230 1791 4586 351 ATOM 107 153 784 117 -3.163 35.911 47.648 1.000 21.87 ARG С ANISOU 784 ARG 117 2269 1865 4178 252 179 9 7 ATOM 785 0 ARG 117 -2.060 35.789 47.102 1.000 22.10 ANISOU 785 0 ARG 117 2197 2270 3931 216 41 2 0 5 ATOM 786 117 -4.682 37.861 47.105 1.000 29.47 CB ARG ANISOU 786 CB ARG 117 2849 1691 6658 -555 - 1 259 ATOM 787 CG ARG 117 -3.485 38.815 47.046 1.000 40.24 ANISOU 787 117 3905 2567 8818 -819 -1330 117 -3.745 40.160 47.716 1.000 52.75 CG ARG -819 -1330 -476 ATOM 788 CDARG ANISOU 788 CD ARG 117 4698 2848 12496 -595 -1653 -1669 ATOM 789 ΝE ARG 117 -3.934 39.987 49.155 1.000 68.00 ANISOU 789 NΞ ARG 117 8247 4719 12872 422 1842 - 3441 ATOM 790 CZARG 117 -3.166 40.448 50.126 1.000 78.38 ANISOU 790 CZ ARG 117 13026 5658 11097 283 448 - 2498 ATOM 791 NH1 ARG 117 -2.097 41.186 49.849 1.000 89.01 ANISOU 791 NH1 ARG 117 14218 11488 8115 -3550 -6761 3577 ATOM 792 NH2 ARG 117 -3.479 40.189 51.391 1.000 82.58 ANISOU 792 NH2 ARG 117 16575 2856 11947 2617 2551 - 2095 ATOM 793 N ILE 118 -3.334 35.759 48.954 1.000 21.70 ANISOU 793 ILE 118 2319 1797 4127 311 271 - 314

- 39 -794 CA ILE 118 -2.206 35.425 49.810 1.000 20.99 ATOM ANISOU 794 CA ILE 118 2546 1624 3805 408 294 - 470 ATOM 795 C ILE ANISOU 795 C ILE 118 -1.596 34.073 49.475 1.000 18.79 118 2222 1534 3384 218 573 - 201 MOTA 796 O ILE 118 -0.409 33.858 49.323 1.000 17.27 O ILE
CB ILE
CB ILE
CG1 ILE ANISOU 796 118 2194 1663 2707 283 351 -136 MOTA 797 118 -2.588 35.542 51.293 1.000 22.62 ANISOU 797 118 2702 1997 3895 276 416 -856 MOTA 798 118 -2.916 36.995 51.700 1.000 27.54 ANISOU 798 CG1 ILE 118 5077 3587 503 768 -401 1801 ATOM 799 CG2 ILE 118 -1.552 34.940 52.206 1.000 23.59 CG2 ILE CD1 ILE ANISOU 799 118 3084 2274 3606 183 254 -818 118 -3.493 37.115 53.096 1.000 29.35 800 MOTA CD1 ILE ANISOU 800 118 5212 2054 3885 558 1114 - 645 119 -2.454 33.069 49.341 1.000 17.93 MOTA 801 N TRP N ANISOU 801 TRP 1605 2828 147 -80 -269 CA TRP MOTA 802 ANISOU 802 CA TRP -25 -16 ATOM 803 C TRP ANISOU 803 C TRP -91 -51 804 O TRP ATOM ANISOU 804 O TRP 119 1892 1674 3113 135 181 6 3 30.690 49.591 1.000 18.32 805 CB TRP 119 -3.127 ANISOU 805 CB TRP 119 2156 3014 - 34 5 - 7 1789 119 -2.934 30.457 51.082 1.000 18.27 ATOM 806 CG TRP ANISOU 806 CG TRP 119 2208 1711 3025 86 349 5 6 ATOM 807 119 -3.354 31.273 52.103 1.000 20.36 CD1 TRP ANISOU 807 CD1 TRP 119 2624 2029 3083 156 276 - 153 808 ATOM CD2 TRP ANISOU 808 CD2 TRP 263 110 ATOM 809 NE1 TRP 119 -2.955 30.773 53.323 1.000 20.55 ANISOU 809 NE1 TRP 119 2471 2229 3109 92 266 - 106 MOTA 810 CE2 TRP 119 -2.260 29.603 53.073 1.000 20.21 ANISOU 810 CE2 TRP 119 2529 2258 2893 180 754 2 9 7 ATOM 811 CE3 TRP 119 -1.576 28.258 51.147 1.000 18.29 ANISOU 811 CE3 TRP 119 2258 1714 2977 42 -70 - 20 119 -1.636 28.728 53.981 1.000 21.97 ATOM 812 CZ2 TRP ANISOU 812 119 2876 2526 2945 384 51 -106 119 -0.968 27.375 52.045 1.000 19.35 CZ2 TRP ATOM 813 CZ3 TRP ANISOU 813 CZ3 TRP 119 2576 2028 2750 187 415 2 9 9 119 -1.026 27.618 53.442 1.000 21.67 CH2 TRP ATOM 814 ANISOU 814 CH2 TRP 119 3033 2379 2823 350 250 9 120 -2.129 32.192 46.701 1.000 16.93 250 9 7 ATOM 815 THR N ANISOU 815 THR Ν ATOM 816 CA THR ANISOU 816 CA THR 817 C ATOM THR 120 2031 1855 2629 241 -155 1 9 2 120 0.700 31.960 44.674 1.000 18.67 120 1996 1887 3212 389 -131 1 7 7 120 -2.487 32.865 44.344 1.000 18.10 120 1951 2204 2720 28 -93 3 4 5 120 -3.773 32.238 44.284 1.000 20.49 ANISOU 817 C THR ATOM 818 0 THR ANISOU 818 O THR MOTE 819 CB THR ANISOU 819 CB THR MOTA 820 OG1 THR 120 1807 2801 3179 59 -363 558 120 -1.919 32.803 42.933 1.000 22.46 120 2438 3266 2830 475 118 7 0 5 121 0.094 33.708 45.956 1.000 18.62 ANISOU 820 OG1 THR MOTA 821 CG2 THR ANISOU 821 CG2 THR MOTA 822 N GLN ANISOU 822 121 2180 1657 3237 123 -94 2 1 3 121 1.466 34.232 45.993 1.000 18.15 121 2077 1698 3119 77 96 5 2 0 121 2.412 33.284 46.718 1.000 17.04 GLN N ATOM 823 CA GLN ANISOU 823 CA GLN MOTA 824 С GLN

- 41 -ATOM 855 CA ASP 124 4.060 30.640 43.544 1.000 17.82 ANISOU 855 CA ASP 124 2103 1747 2921 405 -24 314 MOTA 856 C ASP 124 5.490 30.733 44.024 1.000 17.52 ANISOU 856 C 124 1999 ASP 1439 3219 181 ATOM 857 0 ASP 124 6.402 30.324 43.317 1.000 17.18 ANISOU 857 0 ASP 124 2086 3015 1427 34 181 1 7 7 AASP 124 3.639 MOTA 858 CЭ 31.997 42.942 0.534 21.77 ANISOU 858 CВ AASP 124 3475 2089 2706 642 -372 5 9 7 AASP 124 4.381 MOTA 859 CG 32.304 41.659 0.534 19.28 CG AASP 124 2376 ANISOU 859 1982 2967 173 -553 4 9 5 OD1 AASP 124 4.223 ATOM 860 31.538 40.678 0.534 21.03 OD1 AASP 124 2189 ANISOU 860 2636 3164 -28 76 2 1 OD2 AASP 124 5.068 MOTA 861 33.348 41.639 0.534 24.96 ANISOU 861 OD2 AASP 124 3681 2052 3752 -296 -1067 889 CB BASP 124 3.632 ATOM 862 31.975 42.908 0.466 19.67 CB BASP 124 2559 ANISOU 862 1993 2923 1003 673 446 MOTA 863 BASP 124 2.368 CG 31.849 42.089 0.466 22.78 ANISOU 863 CG BASP 124 3552 3217 1889 872 177 1175 MOTA 864 OD1 BASP 124 2.021 41.545 0.466 27.78 30.781 ANISOU 864 OD1 BASP 124 2138 3932 4483 100 503 347 ATOM 865 OD2 BASP 124 1.703 32.893 41.902 0.466 29.73 ANISOU 865 OD2 BASP 124 3845 3804 3646 1239 -312 1644 MOTA 866 N ARG 125 5.669 31.416 45.153 1.000 16.65 ANISOU 866 N ARG 125 1942 1350 3032 276 139 276 CA ARG ATOM 867 125 7.038 31.528 45.646 1.000 17.58 ANISOU 867 125 1918 1819 2944 98 177 2 4 1 MOTA 868 C 125 7.662 ARG 30.188 45.992 1.000 17.38 ANISOU 868 С ARG 125, 1544 1777 3282 -42 40 273 ATOM 869 0 ARG 125 8.841 29.942 45.754 1.000 18.26 ANISOU 869 125 1639 125 7.062 125 2219 0 ARG 1669 3631 -97 91 - 233ATOM 870 CB ARG 32.468 46.851 1.000 20.45 ANISOU 870 CB ARG 2162 3387 -244 450 - 274ATOM 871 CG ARG 125 6.860 33.916 46.344 1.000 28.23 ANISOU 871 CG ARG 125 3178 2007 5542 147 666 - 222 ATOM 872 CDARG 125 6.693 34.891 47.477 1.000 31.76 ANISOU 872 CD ARG 125 3065 2279 6725 -628 1455 - 993 ATOM 873 NΕ ARG 125 6.496 36.221 46.932 1.000 40.81 ANISOU 873 NΞ ARG 125 3332 2095 10080 -169 1790 -694 MOTA 874 CZARG 125 5.970 37.229 47.628 1.000 43.42 ANISOU 874 CZ ARG 125 4531 2891 9076 839 2072 - 188875 ATOM NH1 ARG 125 5.551 37.025 48.866 1.000 38.62 ANISOU 875 NH1 ARG 125 3999 2858 7816 61 - 700 -858 MOTA 876 125 5.858 NH2 ARG 38.382 47.006 1.000 42.11 ANISOU 876 125 5319 NH2 ARG 2652 8030 908 1627 - 681 ATOM 877 N GLN 126 6.884 29.282 46.557 1.000 15.28 ANISOU 877 GLN 126 1876 N 1527 2404 -70 13 - 60 ATOM 878 CA GLN 126 7.376 27.929 46.853 1.000 15.37 ANISOU 878 CA GLN 126 1726 1625 2488 -54 -31220ATOM 879 С GLN 126 7.649 27.150 45.578 1.000 14.21 ANISOU 879 C GLN 126 1643 1268 2488 -75 -398 7 ATOM 880 0 GLN 126 8.682 26.462 45.496 1.000 15.36 ANISOU 880 0 GLN 126 1531 1554 2753 -37 -316 5 ATOM 881 СЗ GLN 126 6.356 27.158 47.702 1.000 17.40 ANISOU 881 СЗ GLN 126 2034 1313 3264 158 293 4 3 ATOM 882 CG GLN 126 6.336 27.634 49.150 1.000 26.14 ANISOU 882 CGGLN 126 4503 1690 3739 431 1908 - 732 MOTA 883 CDGLN126 5.208 26.998 49.891 1.000 21.95 ANISOU 883 CD GLN 126 2957 2670 2713 0 -123 102 ATOM 884 OE1 GLN 126 4.051 27.372 49.730 1.000 42.52 ANISOU 884 OE1 GLN 126 2994 5747 7416 -62 -1272 3147 ATOM 885 NE2 GLN 126 5.524 26.003 50.691 1.000 28.32

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 ANISOU 885
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                                 3971
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127 7.039
                 TYR
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                                               -41
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                                                     -373 - 36
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             CA TYR
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                                         2277
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                TYR
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                                             7 -84 - 8
 ATOM
        893
            CD2 TYR
 ANISOU 893
            CD2 TYF.
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            CE1 TYR
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127 4.661 25.322 39.071 1.000 15.07
                    127 1450
ATOM
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            CE2 TYR
ANISOU 895
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                                               158
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ATOM
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                                        38.934 1.000 13.71
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ANISOU 896
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127 5.337
127 1682
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            OH
               TYR
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                                        2279
                                               -87
      898 N
                                                     -60 5 3
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ANISOU 898 N
                THR
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ATOM
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                THR
ANISOU 900
           С
                THR
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                                        2466
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ANISOU 911
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ATOM	917	CA	ARG	131 12.163	24.598		1.000 14.91
ANISOU	917	CA	ARG	131 1689	1452	2525	-4 -526 -341
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ATOM	920	CB	ARG	131 11.349	25.316		-109 -170 -230 1.000 15.77
ANISOU		СВ	ARG	131 1720	1613	2660	-54 -493 - 94
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ANISOU		ĊĠ	ARG	131 1703	1695	2711	1.000 15.08 -13 -647 - 141
ATOM	922	CD	ARG	131 9.326	25.390		-13 -647 - 141 1.000 26.56
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ATOM	924	CZ	ARG	131 8.472	27.716		-979 -1682 1413 1.000 31.86
ANISOU		СZ	ARG	131 3546	2861	5697	
ATOM	925		ARG	131 7.467	27.244		-254 -1094 2201 1.000 31.34
ANISOU	925		ARG	131 5127	3636	3144	-1474 -458 -115
ATOM	926		ARG	131 8.633	29.032	30 335	1.000 40.12
ANISOU			ARG	131 3500	2831	8912	-582 -1620 1802
ATOM	927	N	ALA	132 13.893	26.186		1.000 13.42
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ANISOU	933	CA	VAL	133 1902	1566.	2179	120 -491 - 27
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      -287

      137
      1755
      1802
      2493
      83
      -4
      210

      137
      20.926
      19.086
      40.326
      1.000
      15.86

                                         2434
 ATOM
          963
                                                   4938
               OE2 GLU
                                                            -494 531 219
 ANISOU 963 OE2 GLU
          964 N
 ATOM
                                                           -708 -133 1029
                    VAL
 ANISOU 964 N
                    VAL
 ATOM
          965
               CA VAL
                                                                   -287 1 1 3
 ANISOU 965 CA VAL
 ATOM
         966
               C
                    VAL
 ANISOU 966
               С
                          137 1604 1869 2555 -38 -35 6
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 ATOM
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                    VAL
               CB VAL
CB VAL
CG1 VAL
ATOM
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ANISOU 968
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         969
                         137 19.607 17.478 42.176 1.000 16.93
ATOM
ANISOU 969
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MOTA
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         970
                          137 19.144 19.420 43.724 1.000 15.43
                                                           160
               CG2 VAL
                                                                -345 9 6
ANISOU 970
               CG2 VAL
                          137 1529
                                        2090
                                                  2245
ATOM
                          138 20.149 19.407 39.284 1.000 15.52
         971
               N
                                                                  -277 1 8 5
                  LEU
ANISOU 971
               N
                   LEU
                          138 1625
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ATOM
         972
                                                  2535
                                                          -105 -61 109
               CA LEU
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ANISOU 972
              CA LEU
                          138 1576
                                       1862
ATOM
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         973
              С
                          138 21.721 19.396 37.406 1.000 17.42
                                                         -71
                   LEU
ANISOU 973
                         138 1588 2119 2912 -87 162 -
138 22.503 18.609 36.846 1.000 19.13
              С
                   LEU
ATOM
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                   LEU
                                                                  162 - 45
ANISOU 974
              0
                   LEU
                                        2406
ATOM
                                                  2985
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              CВ
                                                          186
                         138 19.211
                   LEU
                                                                  317
                                       19.248 36.996 1.000 14.70
ANISOU 975
              CB
                   LEU
                         138 1592
                                        1642
                                                  2349
        976
                                                          -50
              CG
                         138 17.883
                                                                  141
                   LEU
                                       18.541 37.375 1.000 14.38
ANISOU 976
              CG
                   LEU
                         138 1657
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                                                          -44
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 140 24.357
 20.566
 39.009 1.000 18.77

 140 1742
 2387
 3003 -255 145 6
 ATOM 990 N ALA 3003 -255 145 6 9 39.773 1.000 19.53 3197 -28 ANISOU 990 N ALA 140 1742 MOTA 991 CA ALA 140 25.532 20.169 ANISOU 991 CA ALA 140 1583 2641 ATOM 992 C ALA 140 25.932 18.732 39.490 1.000 18.96 ANISOU 992 C ALA 140 2018 2342 2843 -67 76 - 103 ATOM 993 0 ALA 140 27.109 18.335 39.626 1.000 21.36 ANISOU 993 0 ALA 140 1900 2436 3778 -2 472 - 80 CB ALA 140 25.273 20.345 41.275 1.000 19.74 ATOM 994 ANISOU 994 CВ ALA 140 1824 2592 3084 35 0 - 360 995 THR 141 24.958 17.943 39.062 1.000 20.32 ATOM N ANISOU 995 N THR 141 2014 2209 3498 -115 305 -138 CA THR MOTA 996 141 25.151 16.530 38.717 1.000 17.15 CA THR ANISOU 996 141 1870 2039 141 25.269 16.278 2609 61 51 2 1 8 MOTA 997 С THR 37.208 1.000 17.44 ANISOU 997 С 141 1492 2443 141 25.343 15.106 THR 2693 21 278 1 9 9 ATOM 998 0 THR 36.792 1.000 19.24 ANISOU 998 0 THR 141 1871 2623 2814 63 579 - 63СВ ATOM 999 THR 141 24.048 15.629 39.290 1.000 16.79 141 1708 2261 141 22.788 16.012 141 1894 2235 141 23.982 15.734 ANISOU 999 CBTHR 2410 83 164 3 1 1000 OG1 THR ATOM 38.710 1.000 17.18 ANISOU 1000 OG1 THR 2399 -101 -53 518 1001 CG2 THR 40.807 1.000 17.83 ANISOU 1001 CG2 THR 141 1521 2878 2377 164 -43 2 0 142 25.361 17.301 MOTA 1002 N GLY 36.381 1.000 19.69 ANISOU 1002 N 142 2091 GLY 2789 .2603 -708 302 297 1003 CA GLY ATOM 142 25.517 17.123 34.923 1.000 19.08 ANISOU 1003 CA ${ t GLY}$ 142 1878 2819 2551 128 -163 2 5 5 ATOM 1004 C GLY 142 24.284 16.441 34.313 1.000 18.75 ANISOU 1004 C GLY 142 1972 2410 2744 0 252 - 117 ATOM 1005 0 GLY 142 24.443 15.755 33.315 1.000 22.41 ANISOU 1005 O GLY 142 2432 2681 3403 -161 571 -680 ATOM 1006 N THR 143 23.093 16.650 34.854 1.000 17.28 ANISOU 1006 N THR 143 1895 2002 2667 67 300 2 4 4 ATOM 1007 CA THR 143 21.909 15.932 34.393 1.000 16.88

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- 46 -
 ANISOU 1007 CA THR 143 1953 2006
                                                       2456
                                                               164
                                                                       332 6 6
 ATOM
           1008 C
                    THR 143 20.998 16.660 33.432 1.000 17.02
 ANISOU 1008 C
                      THR 143 2149 1795
                                                       2521
                                                               82 196 1 1 7
 ATOM
           1009 0
                      THR 143 20.457 17.713 33.764 1.000 20.30
 ANISOU 1009 O
                      THR
                            143 2795
                                            1815
                                                      3103
                                                               344
                                                                       12 - 28
                            143 21.085 15.490 35.623 1.000 16.40
 ATOM
           1010 CB
                     THR
 ANISOU 1010 CB
                            143 1755
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 ANISOU 1011 OG1 THR
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          1012 CG2 THR
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                     THR 143 1957 2290 3167 -192 -94 1
GLU 144 20.742 16.070 32.248 1.000 18.79
GLU 144 2138 2203 2800 47 12 -1 21
GLU 144 19.729 16.573 31.334 1.000 20.13
 ANISOU 1012 CG2 THR
                                                               -192 -94 100
 MOTA
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 ANISOU 1013 N
 MOTA
          1014 CA GLU
 ATOM 1014 CA GLU 144 2202 2696 2750 -292 -41 3 1 6
ATOM 1015 C GLU 144 18.637 15.506 31.254 1.010 19.18
          1015 C GLU 144 2255 2614 2418 -292 230 -131 1016 O GLU 144 18.827 14.433 30.665 1.000 21.46 1017 CB AGLU 144 20.250 17.061 30.006 0.753 29.50
 ATOM
 ANISOU 1016 O
 ATOM
ANISOU 1017 CB AGLU 144 3376 4266 3566 -855 206 1501 ATOM 1018 CG AGLU 144 20.195 18.567 29.741 0.753 36.54 ATOM 1019 CD AGLU 144 6059 3913 3913 -1728 1769 7 9 5 ATOM 1019 CD AGLU 144 21.242 19.411 30.426 0.753 33.13
ANISOU 1019 CD AGLU 144 4189 3432
ANISOU 1019 CD AGLU 144 4189 3432 4966 104 744 8 8 4
ATOM 1020 OE1AGLU 144 21.079 19.690 31.641 0.753 51.91
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ANISOU 1022 CB BGLU 144 20.372 16.724 29.951 0.247 18.36
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         1023 CG BGLU 144 21.214 17.988 29.779 0.247 23.54
ATOM
ANISOU 1023 CG BGLU 144 1301 3586 4056 -38 595 5
ATOM 1024 CD BGLU 144 21.150 18.468 28.336 0.247 33.24
                                                     4056 -38 595 558
ATOM 1024 CD BGLU 144 3589 3975 5064 438 -20 26
ANISOU 1024 CD BGLU 144 3589 3975 5064 438 -20 26
ATOM 1025 OE1BGLU 144 20.417 17.818 27.557 0.247 28.68
                                                              438 -20 2031
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ATOM
ANISOU 1026 OE2BGLU 144 3176
ATOM 1027 N PRO 145 17.508
ANISOU 1027 N PRO 145 2132
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                           145 2132 1825
ATOM 1028 CA PRO
ANISOU 1028 CA PRO
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ANISOU 1029 C
                    PRO
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ATOM · 1031 CB
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                          MOTA
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ANISOU 1032 CG
                    PRO
ATOM
         1033 CD
                    PRO
ANISOU 1033 CD PRO
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ATOM
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ANISOU 1034 N
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ATOM
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ANISOU 1035 CA ASP
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ATOM
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ASP 146 12.959 14.333 29.422 1.000 18.29
ASP 146 2491 2173 2287 -168 203 -
ANISOU 1036 C
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ATOM
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ANISOU 1037 O
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- 47 -1038 CB ASP 146 14.221 11.735 28.717 1.000 23.50 ATOM 1038 CB ASP 146 3489 1671 3769 -653 908 -61039 CG ASP 146 13.636 11.508 27.334 1.000 34.15 ANISOU 1038 CB 3769 -653 908 -665 ANISOU 1039 CG ASP 146 4070 4205 4700 -1004 361 -2386 1040 OD1 ASP 146 12.393 11.521 27.138 1.000 44.73 ANISOU 1040 OD1 ASP 146 3971 9175 3849 -2156 683 3 7 8 1041 OD2 ASP 146 14.421 11.229 26.397 1.000 44.78 1041 OD2 ASP 146 4342 8626 4046 -813 289 -ANISOU 1041 OD2 ASP 146 4342 8626 4046 -813 289 -7 ATOM 1042 N GLY 147 13.901 14.854 27.450 1.000 19.28 ANISOU 1042 N GLY 147 2622 2331 2374 -635 -72 1 ATOM 1043 CA GLY 147 12.916 15.878 27.171 1.000 18.58 ANISOU 1043 CA GLY 147 2463 2607 1991 -550 -234 - ATOM 1044 C GLY 147 13.355 17.262 27.590 1.000 18.25 289 -2326 -72 113 ANISOU 1043 CA GLY 147 2463 2607 1991 -550 -234 - 3 6 ATOM 1044 C GLY 147 13.355 17.262 27.590 1.000 18.25 ANISOU 1044 C GLY 147 12.586 18.183 27.289 1.000 20.74 ANISOU 1045 O GLY 147 2469 2739 2673 -182 -144 2 0 5 ATOM 1046 N GLY 148 14.494 17.357 28.286 1.000 17.38 ANISOU 1046 N GLY 148 2237 2174 2191 -462 -42 - 9 0 ATOM 1047 CA GLY 148 2307 1789 2255 39 -82 - 77 ANISOU 1047 CA GLY 148 14.653 1789 2255 39 -82 - 77 ANISOU 1048 C GLY 148 13.637 18.658 28.672 1.000 16.72 ANISOU 1049 O GLY 148 13.637 18.654 30.694 1.000 16.29 ATOM 1050 N VAL 149 15.431 20.003 30.641 1.000 16.29 ATOM 1050 N VAL 149 15.431 20.003 30.641 1.000 14.93 ANISOU 1051 CA VAL 149 15.431 20.003 30.641 1.000 14.93 ANISOU 1051 CA VAL 149 15.275 20.509 32.017 1.000 14.16 ANISOU 1052 C VAL 149 13.203 ANISOU 1052 C VAL 149 13.203 ANISOU 1055 CGI VAL 149 16.238 1044 2682 -39 83 1 8 8 ATOM 1053 O VAL 149 16.33 1517 2390 -160 -40 1 0 7 ATOM 1055 CGI VAL 149 16.238 22.101 33.752 1.000 14.03 ANISOU 1055 CGI VAL 149 16.238 22.101 33.752 1.000 17.85 ANISOU 1055 CGI VAL 149 16.238 22.101 33.752 1.000 17.85 ANISOU 1055 CGI VAL 149 16.238 22.101 33.752 1.000 17.85 ANISOU 1055 CGI VAL 149 16.238 22.101 33.752 1.000 17.85 ANISOU 1055 CGI VAL 149 16.238 22.101 33.752 1.000 17.85 ANISOU 1055 CGI VAL 149 16.238 22.101 33.752 1.000 17.85 ANISOU 1055 CGI VAL 149 16.238 22.101 33.752 1.000 17.85 ANISOU 1056 CG2 VAL 149 17.733 20.614 22.199 31.371 1.000 17.85 ANISOU 1056 CG2 VAL 149 1618 1937 22.600 32.417 1.000 17.85 ANISOU 1057 N GLU 150 13.634 22.199 31.371 1.000 17.85 ANISOU 1057 N GLU 150 13.634 22.199 31.371 1.000 17.85 ANISOU 1058 CA GLU 150 12.471 23.028 31.687 1.000 14.91 ANISOU 1058 CA GLU 150 12.471 23.028 31.687 1.000 14.91 ANISOU 1058 CA GLU 150 12.471 23.028 31.687 1.000 14.91 ANISOU 1058 CA GLU 150 12.471 23.028 31.637 1.000 14.91 -234 - 36150 1759 1328 2711 186 36 267 150 12.471 23.028 31.687 1.000 14.91 150 1591 1434 2640 93 13 4 1 5 150 11.182 22.237 31.553 1.000 16.66 150 1680 1980 2670 -197 113 1 99 150 10.259 22.408 32.379 1.000 15.89 150 1697 1761 2578 29 79 5 8 0 150 12.531 24.305 30.874 1.000 17.07 150 1925 1337 3223 254 189 5 1 3 150 13.761 25.167 31.220 1.000 19.00 150 2483 1212 3523 -65 -95 4 6 5 150 13.810 25.624 32.658 1.000 20.32 150 2444 1746 3532 -130 -24 4 5 4 150 12.781 25.749 33.377 1.000 20.88 150 2558 1728 3648 29 58 3 9 6 150 14.913 25.946 33.161 1.000 21.77 150 2549 2030 3693 -165 -202 2 7 3 151 11.050 21.288 30.603 1.000 14.98 1058 CA GLU ANISOU 1058 CA GLU ATOM 1059 C GLU ANISOU 1059 C GLU ATOM 1060 O GLU ANISOU 1060 O GLU 1061 CB GLU 1061 CB GLU ATOM ANISOU 1061 CB 1062 CG ATOM GLU ANISOU 1062 CG GLU 1063 CD ATOM GLU ANISOU 1063 CD GLU MOTA 1064 OE1 GLU ANISOU 1064 OE1 GLU MOTA 1065 OE2 GLU ANISOU 1065 OE2 GLU 150 2549 2030 3693 -165 -202 2 7 3 ATOM 1066 N ALA 151 11.050 21.288 30.603 1.000 14.98 ANISOU 1066 N ALA 151 1649 1710 2334 37 -307 5 5 1 ATOM 1067 CA ALA 151 9.834 20.475 30.543 1.000 15.79 ANISOU 1067 CA ALA 151 1820 2045 2136 -173 -198 4 0 8 ATOM 1068 C ALA 151 9.748 19.531 31.724 1.000 15.38 ANISOU 1065 OE2 GLU

•						4.0			
ANISOU ATOM	1069	0	ALA ALA	151 151	1674 8.642	-48- 1953 19.186	2216 32 184	165	181 442 16.51
ANISOU ATOM	1070	CB	ALA ALA	151 151	1778	1852 19.663	2643	-152	110 330
ANISOU ATOM	1071	N	ALA PHE	151 152	1910 10.893	2811 19.135	2139	-275	-316 1 6 6 14.25
ANISOU ATOM	1072	CA	PHE PHE	152 152	10.893	1132 18.285	2423	10 -1	07 263
ANISOU ATOM	1073	С	PHE	152 152	10.406	1291 19.056	2353 34.695	-102	-34 304
ANISOU ATOM ANISOU	1074	0	PHE	152 152	1481 9.679	1400 18.495	2412 35.558	-43	-165 1 9 6 14.50
ATOM ANISOU	1075 1075	СВ	PHE PHE PHE	152 152	1590	1482 17.744	2438 33.728	-85 1.000	25 2 6
ATOM ANISOU	1076	CG	PHE PHE	152 152 152	1504 12.475 17 ₄ 7	1547 16.966	2248 35.011	-29 1.000	$111 4 \in 3$ 14.04
ATOM ANISOU	1077 1077	CD1	PHE		12.032 1906	1386 15.653 1306	2200 35.076	1.000	8 2 4 7
ATOM ANISOU	1078 1078	CD2	PHE PHE		13.094 1927	17.499 1770	2069 36.127 2259	165 1.000 -155	-36 281 15.67
ATOM ANISOU	1079 1079	CE1	PHE	152 152	12.213 1669	14.949 1507	36.263 2165		-115 2 3 3 1 4 . 0 6 -282 3 4 7
ATOM ANISOU ATOM	1080	CE2	PHE	152	13.323 1724	16.799 1671		1.000 35 -1	14.83
ANISOU ATOM	1081 1081 1082	CZ	PHE	152	12.861	15.522 1734	1916	1.000 -162	14.86 99 113
ANISOU ATOM	1082	N	LEU LEU LEU	153	10.789 1742 10.454	20.324	34.789 2696	58 11	15.25 0 154
ANISOU ATOM		CA	LEU LEU	153	1783 9.082	21.151 1429 21.791	35.939 2354	-66	14.65 16 2 0 3
ANISOU ATOM	1084 1085	C 0	LEU LEU	153 153	1732	1402 22.216	35.877 2362 36.953	-80	14.47 76 1 1
ANISOU ATOM	1086	СВ	LEU LEU	153 153	1940 11.537	1454 22.224	2616 36.165	-313	312 - 157 16.53
ANISOU ATOM	1086	CG	LEU LEU	153	1626 12.914	1451 21.685	3205 36.514	-23	269 - 83
ANISOU ATOM ANISOU	1087	CD1	LEU LEU	153 153	1893 13.922	2013 22.829	2135 36.614	-33	-186 - 36
ATOM ANISOU	1089	CD2	LEU	153	1732 12.863		2791 37.794	-156 1.000	80 - 876
ATOM ANISOU	1090	N	ASP ASP	154	3083 8.473 1768	3182 21.866	2005	365	261 193 14.41
ATOM ANISOU	1091 1091	CA	ASP ASP	154	7.092 1665	1181 22.373 1615	2525 34.553 2760	-25 1.000	-8 2 9 3 15.90
	1092 1092	C C	ASP ASP	154	6.216 1859	21.161 1304	34.814 2409	-195 1.000 -92	27 7 6 9 14.66 143 5 1 5
ATOM ANISOU	1093	0	ASP ASP	$\begin{array}{c} 154 \\ 154 \end{array}$	5.995 2561	20.368 1455	33.889 2557		17.30
ATOM ANISOU ATOM	1094 1094 1095	CB	ASP ASP	154	6.923 1905	22.909 2077	33.125 3081	1.000	18.59 269 1317
ANISOU ATOM	1095	CG	ASP ASP	154	5°.461 2029 4.561	23.157 2531	32.768 2990	226	129 1436
ANISOU ATOM	1096 1097	OD1 OD2	ASP ASP	154	1949 5.207	23.253 2209 23.189	33.639 3318	92 223	1496
ATOM	1097 1098	OD2	ASP CYS	154	2512 5.831	3475 20.904	31.554 3029 36.070	246	-137 653
ANISOU	1098	N	CYS	155	1708	1365	2342	-101	14.25 -62 546

- 49 -1099 CA CYS MOTA 155 5.418 19.569 36.468 1.000 13.45 ANISOU 1099 CA CYS 155 1608 1346 2158 -191 4 458 ATOM 1100 C CYS 155 4.157 19.574 37.302 1.000 12.49 ANISOU 1100 C CYS 155 1644 1331 1772 -200 -148 6 2 1101 0 CYS 155 3.224 20.303 36.941 1.000 14.55 ANISOU 1101 O CYS 155 1633 1492 2402 -122 -111 4 4 2 ATOM 1102 CB 155 6.664 CYS 18.872 37.098 1.000 14.37 ANISOU 1102 CB 155 1907 CYS 1366 2186 122 -137211ATOM 1103 SG 155 7.265 CYS 19.595 38.641 1.000 14.99 ANISOU 1103 SG CYS 155 1561 1821 2315 -74 -98 182 ATOM 1104 N GLU 156 4.060 18.706 38.316 1.000 12.89 ANISOU 1104 N GLU 156 1575 1379 -130 29 1 9 4 1945 ATOM 1105 CA GLU 156 2.788 18.447 39.029 1.000 12.98 ANISOU 1105 CA GLU 156 1508 1311 2114 -210 21 1 4 0 ATOM 1106 C GLU 156 2.987 18.676 40.510 1.000 12.34 ANISOU 1106 C GLU 156 1414 1198 2078 102 24 204 ATOM 1107 O GLU 156 2.828 17.757 41.289 1.000 14.89 ANISOU 1107 O GLU 156 1875 1425 2359 -15 -54 442 ATOM 1108 CB GLU 156 2.278 17.047 38.678 1.000 14.48 ANISOU 1108 CB GLÜ 156 1968 1323 2213 -279 120 8 7 1109 CG ATOM GLU 156 1.855 17.038 37.227 1.000 14.86 ANISOU 1109 CG GLU 156 1894 1526 2227 -120 95 - 152 MOTA 1110 CD GLU 156 0.523 17.687 36.932 1.000 17.10 ANISOU 1110 CD 156 2091 GLU 1976 2431 44 -4 1 4 4 1111 OE1 GLU ATOM 156 -0.204 17.967 37.886 1.000 17.98 ANISOU 1111 OE1 GLU 2155 156 1811 2866 -35 10 - 355 ATOM 1112 OE2 GLU 156 0.214 17.990 35.759 1.000 20.99 ANISOU 1112 OE2 GLU 156-2854 2419 2704 -386 -516 5 6 2 ATOM 1113 N 157 3.292 PRO 19.893 40.958 1.000 12.09 ANISOU 1113 N 157 1314 157 3.576 PRO 1347 1934 12 -48 2 4 9 1114 CA PRO ATOM 20.121 42.391 1.000 13.28 ANISOU 1114 CA PRO 157 1425 1696 1924 -68 117 147 ATOM 157 2.330 1115 C PRO 19.996 43.248 1.000 12.87 ANISOU 1115 C PRO 157 1236 1737 1916 -214 -47 124 ATOM 1116 0 PRO 157 1.192 42.744 1.000 13.73 20.190 ANISOU 1116 O 157 1286 PRO 1717 2214 -190 -17 143 157 4.061 ATOM 1117 CB PRO 21.580 42.407 1.000 13.94 ANISOU 1117 CB PRO 157 1518 1729 2047 -289 -166 2 4 7 ATOM 1118 CG PRO 157 3.363 22.184 41.226 1.000 13.06 ANISOU 1118 CG PRO 157 1558 1518 1887 -32 -158 - 881119 CD ATOM PRO 157 3.494 21.128 40.167 1.000 12.03 ANISOU 1119 CD PRO 157 1521 1081 1968 -2 -7 1 2 1 ATOM 1120 N LEU 158 2.542 19.738 44.526 1.000 13.02 ANISOU 1120 N LEU 158 1554 1493 1899 -124 148 MOTA 1121 CA LEU 158 1.438 19.699 45.496 1.000 12.72 ANISOU 1121 CA LEU 1552 158 1465 1815 -126 -14 ATOM 1122 C LEU 158 1.927 20.389 46.772 1.000 12.90 ANISOU 1122 C LEU 158 1230 1715 -27 1957 -29 -80 ATOM 1123 0 LEU 158 2.975 19.977 47.289 1.000 14.06 ANISOU 1123 O 158 1374 LEU 1666 59 - 257 - 236 2304 ATOM 1124 CB 158 1.046 LEU 18.244 45.815 1.000 13.58 ANISOU 1124 CB 158 1673 LEU 1590 1896 -213 57 171 ATOM 1125 CG LEU 158 0.044 18.030 46.945 1.000 14.84 ANISOU 1125 CG LEU 158 1471 1774 2396 -16 262 242 MOTA 1126 CD1 LEU 158 -1.333 18.635 46.671 1.000 16.96 ANISOU 1126 CD1 LEU 158 1485 2196 2764 5 -148 -401 ATOM 1127 CD2 LEU 158 -0.142 16.539 47.161 1.000 14.98 ANISOU 1127 CD2 LEU 158 1976 1820 1897 -390 171 7 9 ATOM 1128 N LEU 159 1.139 21.306 47.283 1.000 13.44 ANISOU 1128 N LEU 159 1509 1434 2165 43 -87 -119 MOTA 1129 CA LEU 159 1.443 21.963 48.571 1.000 13.39

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			- 52 -			
ANISOU 1205 ATOM 1206 ANISOU 1206 ATOM 1207 ANISOU 1207 ATOM 1208 ATOM 1209 ANISOU 1209 ATOM 1210 ANISOU 1210 ATOM 1211 ANISOU 1211 ATOM 1211 ATOM 1212 ANISOU 1212 ATOM 1213 ANISOU 1213 ATOM 1214 ANISOU 1214 ANISOU 1215 ATOM 1215 ANISOU 1216 ANISOU 1216	PHE PHO PRO PRO PRO PRO PRO PRO PRO PRO PRO PR	164 1.494 164 1.494 165 3.876 165 3.299 165 3.299 165 3.882 165 3.882 165 3.882 165 3.882 165 3.892 165 3.695 165 3.695 165 3.192 178 7.297 178 8.2297 178 8.2297 178 8.2297 178 8.2297 178 8.1277 178 8.2297 178 8.2297 178 8.2297 178 8.2297 178 8.2297 178 10557 178 8.2297 178 8.2297 178 8.2297 178 10557 178 9.665 178 10.633 178 11.470 178 9.662 178 10.633 179 1.8879 179 7.356 179 7.356 179 7.366 179 7.366 179 7.366 179 7.366 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.3838 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384 179 7.384	41707.00.64.45.41.61.94.40.3 3 0 9 9 2 2 0 0 9 7 0 8 8 9 9 3 8 8 9 2 0 0 9 9 2 2 0 0 9 7 0 8 1 0 0 9 7 0 8 1 0 0 9 7 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	4172 3751 66.375.80 67.80 68.877.80 68.87.80 68.87.80 68.87.80 68.87.80 68.87.80 68.99.70 68.99.70 68.99.70 68.99.70 68.99.70 68.99.70 68.99.70 68.99.70 68.99.70 68.99.70 68.99.70 69.7	220 501 3 8 1.000 38.44 -765 271 8 2 1.000 35.82 5 688 - 828 1.000 33.9(-1149 194 1 6 1.000 64.52 278 -218 3 7 1.000 43.31 -984 -2821 - 1.000 47.36 -2598 -1186 1 1.000 56.53 -4835 1265 - 6 1.000 55.55 -1314 -1197 - 1.000 62.34 -1971 194 - 4 1.000 54.23 1878 -3799 5 1.000 66.44 -1170 4090 - 5 1.000 52.90 102 1230 10 1.000 52.90 102 1230 10 1.000 55.25 -946 2260 - 1 1.000 55.25 -946 2260 - 1 1.000 58.51 -1820 3675 - 2 1.000 41.49 -155 1916 11 1.000 43.15 90 1338 5 3 0 1.000 47.63 195 860 - 5 1.000 52.00 1669 -1168 - 1.000 59.74 3628 -2691	85 08 34 7 7 9 21 135 204 02 1822 43 11 16 31 83 134 851 37
ANISOU 1214 ATOM 1215	NE ARG CZ ARG	179 7384 179 1.322	7834 14.470	4539 66.556	1669 -1168 - 1.000 64.81	
ATOM 1216 ANISOU 1216 ATOM 1217 ANISOU 1217	NH1 ARG NH1 ARG NH2 ARG NH2 ARG	179 1.637 179 9535 179 0.907 179 10451	14.518 8090 15.606 9083	65.268 5074 67.117 5478	1.000 59.74 3628 -2691 4 1.000 65.83 4171 -776 12	145
ATOM 1218 ANISOU 1218 ATOM 1219 ANISOU 1219	N MET	180 5.304 180 5383 180 5.264	9.501 3769 9.035	7550 62.210	1.000 40.44	245
ATOM 1220 ANISOU 1220	C MET	180 2356 180 6.552 180 2731	5467 8.258 6220	7543 61.920 7733	-398 574 -1 1.000 43.91 18 320 -2324	

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ANISOU		-	MET		2377	5064			
							7554	-395	906 - 912
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ANISOU	1222	СВ	MET	130	2749	7966	8223	-452	-1114 7 2
ATOM	1223	CG	MET	180	5.339	9.818	59.757		
ANISOU			MET		7280	0011	7587		
						8911 11.015	7587	-2331	-3353 -505
ATOM	1224		MET		4.622	11.015	58.608		
ANISOU			\mathtt{MET}		7480	13510	7216	4918	-262 - 905
$\mathtt{MOT}A$	1225	CΞ	MET	180	4.501	10.037	57.110	1 000	79 59
ANISOU	1225	CE	MET		6119	20000	4120		1874 - 912
ATOM	1226		ALA		6.376	7.112		1 000	10/4 - 917
ANISOU						7.112		1.000	3 / . 4 4
			ALA		3523	5646	5055	-271	882 -1132
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ANISOU	1227	CA	ALA	181	3980	3980	6250	-625	2048 4 6 1
MOTA	1228	С	ALA		8.287	6 591	59 837	1 000	31 /0
ANISOU			ALA		2975	3042	5149	2.000	
ATOM	1229		ALA			3842	5149	-32	920 956
					7.834	7.393 4021	58.997	1.000	
ANISOU			ALA		2903	4021		197	-93 164
\mathtt{ATOM}	1230		ALA		6.727	4.817	60.620	1.000	42.66
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ATOM	1231	N	PRO		9.541	6 137	59.840		
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ATOM	1232		PRO			4431	2296	-240	-76 320
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ATOM	1234	0	PRO	182	9.448	5.326	57.080		
ANISOU	1234	Ô	PRO		2991	2496	2759	-440	-340 - 55
ATOM	1235		PRO		11.768	2486 5.939 3860	2/39		
ANISOU						5.939	59.047		
			PRO		2589	3860	3042	-170	-286 1 5 3
ATOM	1236		PRO		11.681	5.351 3582 5.210	60.393	1.000	28.42
ANISOU			PRO	182	3352	3582	3863	656	321 1038
ATOM	1237	CD	PRO		10.215	5.210	60.747		
ANISOU			PRO		3333	4905	4000	-826	
ATOM	1238		HIS		10.111	7 /1/	4 000		
ANISOU				100	20.111	7.414	56.561	1.000	19.27
			HIS		2131	7.414 2658 7.306	2533		-204 1 7 6
ATOM	1239		HIS		9.757	7.306	55.144	1.000	18.01
ANISOU			HIS		1882	2311	2652	-341	-455 3 4 6
ATOM	1240		HIS	183	10.749	8.124 1560	54.337	1,000	15.74
ANISOU	1240	С	HIS		1964	1560	2456	-75	-352 1 2 8
ATOM.	1241		HIS	183	11 355	9.061	54 959	1 000	1 2 1 4
ANISOU			HIS	103	2297	2093	24.000	1.000	100 10C
				100	4471 0 330	2033	2504	-509	-127 - 135
ANTON	1040	CD	UTD	T 8 7	0.338	7.781			
ANISOU			HIS		1970	2173	2945		-243 3 7 1
ATOM	1243		HIS		8.089	9.120	55.447	1.000	26.67
ANISOU	1243	CG	HIS	183	3100	2751	4281	262	222 - 306
ATOM	1244	ND1	HIS		7.884	9.362	56.800		
ANISOU				103	4432				
ATOM	1245			100	4432	4078	4926		1466 - 1454
	1242	CDZ	uis		8.051	10.311	54.821		
ANISOU					4117	2522	5898	1687	-677 -173
ATOM	1246	CE1	HIS	183	7.739	10.658	56.980	1.000	35.91
ANISOU	1246	CE1	HIS		2611		6565	-472	
ATOM	1247	NE2	HIS		7.829	11.251	55.798		
ANISOU	1247	MES	HTC		4375				
ATOM	1247	NT NT				3417	7614		-1013 -1590
			TYR		10.890	7.778	53.061		
ANISOU			TYR		1973	1551	2434	-124	-470 1 0 7
MOTA	1249		TYR	184	11.605	8.685	52.152		
ANISOU	1249	CA	TYR		1798	1392	2438	147	-312 1 4 5
ATOM	1250		TYR		10.572	9.239			14.53
ANISOU			TYR		1656				
ATOM						1449	2416	-70	-399 9 8
A I ON	1251	J	TYR	⊥84	9.468	8.728	51.045	1.000	15.83

					- 54 -			
ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU	1254 C 1254 C 1255 C	B TYR B TYR G TYR G TYR C TYR D1 TYR D1 TYR	184 184 184 184	1717 12.699 1686 12.383 1743 12.200 1549 12.329	1383 8.004 1323 6.785 1313 5.540 1315 6.836	2943	69 -3 1.000 109 1.000 -29	15.66 66 - 168 14.85 -567 4 3 15.49 -575 190
ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM	1256 C 1256 C 1257 C 1257 C 1258 C 1258 C 1259 O	E1 TYR E1 TYR E2 TYR E2 TYR E2 TYR E TYR E TYR E TYR	184 184 184 184 184 184	1724 11.962 1695 12.130 2340 11.915 1695 11.682	1763 4.396 1244 5.661 1776 4.449 1736 3.325	2552 50.442 2992 48.447 2540 49.083 3014 48.310	55 - 2 1.000 229 1.000 4 83 1.000 -156	7 - 6 4 15.61 -137 1 1 3 17.52 - 9 0 16.96 -480 3 4
ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM	1260 N 1260 N 1261 C 1261 C 1262 C 1262 C 1263 O	ASP ASP A ASP ASP ASP ASP	184 185 185 185 185 185	2020 10.924 1518 10.026 1875 10.240 1182 11.357	1775 10.330 1599 11.005 1322 10.490 1385 10.135	3352 50.502 2338 49.574 2078 48.152 2211 47.824	260 1.000 87 -22 1.000 141 1.000 -160	-277 - 3 1 2 1 4 . 3 6 25 2 7 6 1 3 . 8 8 -364 - 4 2 1 2 . 5 7 -77 - 1 3 0
ATOM ANISOU ATOM	1265 C 1265 C 1266 O	B ASP B ASP G ASP G ASP D1 ASP D1 ASP D2 ASP	185 185 185 185 185 185 185	1177 10.294 1879 9.702 2680 9.507 3553 9.174	1637 12.521 1293 13.155 1659 12.466 3133 14.257	2559 49.580 2517 50.830 2351 51.856 2314 50.742	121 1.000 232 1.000 443 1.000	-186 - 159 17.61 -13 - 172 23.69 -302 5 2 1 24.32
ATOM ANISOU ATOM ANISOU ATOM	1268 N 1269 C 1269 C 1270 C 1270 C 1271 O	LEU LEU A LEU LEU LEU LEU LEU	186 186 186 186	4063 9.141 1271 9.169 1533 9.134 1730 8.971 3721	1730 10.465 1378 10.091 1225 11.292 1307 11.173	3449 47.382 2126 45.986 2150 45.052 2330 43.849	-117 1.000 -331 1.000 -93 1.000	-117 -117 12.92 -84 -175 14.12 -165 5 5 20.12
ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU	1272 C 1272 C 1273 C 1273 C 1274 C 1274 C 1275 C 1275 C	B LEU B LEU G LEU G LEU D1 LEU D1 LEU D2 LEU D2 LEU	186 186 186 186 186 186	8.040 1509 8.020 1549 6.929 1686 9.369 1689	1643 9.106 1310 7.811 1141 6.908 1845 7.115	2280 45.609 2393 46.438 3361 45.866 3825 46.341 3528	-270 1.000 -145 1.000 -700	-375 - 6 15.92 -307 168 19.36 -209 3 9 6
ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU	1276 N 1276 N 1277 C 1277 C 1278 C 1278 C 1279 O 1279 O	SER SER SER SER SER SER SER SER	187 187 187 187 187 187 187	9.286 1326 9.388 1489 10.736 1482 11.683 1532	12.494 1234	45.618 2608 44.826	1.000 -26 1.000 -54 1.000 -17 1.000	13.60 -95 137 13.22 -68 2 9 12.79 -114 - 9 0
ATOM ANISOU ATOM ANISOU	1281 0	B SER	187	9.201 1463 10.296 1589	14.915 1282 14.873 1420	45.811 2147 46.716 2015	1.000 164	12.87 -154 9 8

- 55 -MOTA 1282 N MET 188 10.898 14.844 43.292 1.000 13.44 ANISOU 1282 N MET 188 1552 1334 2221 -64 -34 - 26 1283 CA MET MOTA 15.380 188 12.215 42.878 1.000 12.11 ANISOU 1283 CA MET 188 1508 1261 1833 29 -60 - 61 1284 C MOTA MET 188 12.853 16.022 44.104 1.000 12.78 ANISOU 1284 C ATOM 1285 O MET 188 1563 1156 2136 167 -311 - 42MET 188 13.896 15.550 44.600 1.000 13.40 ANISOU 1285 O MET 188 1408 1390 2294 116 -264 - 261286 CB MET MOTA 188 12.038 16.300 41.667 1.000 13.66 ANISOU 1286 CB MET 188 1565 1501 44 -161 2123 2 0 7 188 13.296 17.095 41.315 1.000 14.05 ATOM 1287 CG MET ANISOU 1287 CG 188 1697 MET 1595 2046 66 150 1 3 3 ATOM 1288 SD MET 188 14.600 15.971 40.752 1.000 14.96 ANISOU 1288 SD 188 1565 MET 1591 2529 109 -81 110 188 16.005 17.102 40.686 1.000 17.74 ATOM 1289 CE MET ANISOU 1289 CE MET - 188 1852 2032 189 12.244 17.112 44.616 1.000 12.62 189 1586 1203 2007 103 2855 -242 505 121 ATOM 1290 N VAL ANISOU 1290 N VAL -147 - 134ATOM 1291 CA VAL 189 12.565 17.671 45.918 1.000 12.60 ANISOU 1291 CA VAL 189 1412 1438 1937 -228 -11 -44 ATOM 1292 C 189 11.285 17.968 46.679 1.000 11.71 VAL ANISOU 1292 C VAL 1.89 1328 1294 1825 -170 -171 - 4 9 ATOM 1293 O 189 10.227 18.099 VAL 46.050 1.000 12.56 ANISOU 1293 O 189 1446 VAL 1291 2036 21 -320 - 49 45.856 1.000 12.95 MOTA 1294 CB VAL 189 13.440 18.955 ANISOU 1294 CB VAL 189 1150 1517 2252 -174 - 20594189 14.778 18.637 189 1376 2094 MOTA 1295 CG1 VAL 45.167 1.000 15.54 ANISOU 1295 CG1 VAL 2437 -140 161 9 1 189 12.730 20.056 MOTA 1296 CG2 VAL 45.082 1.000 15.00 ANISOU 1296 CG2 VAL 189 1763 1391 2547 -130 -483 8 1 ATOM 1297 N THR 190 11.425 18.067 47.984 1.000 12.18 ANISOU 1297 N THR 190 1445 1422 1760 -109 -130 1 0 ATOM 1298 CA THR 190 10.353 18.454 48.897 1.000 11.98 ANISOU 1298 CA THR 190 1292 1356 1903 -57 -221 - 151 ATOM 1299 C THR 190 10.879 19.630 49.710 1.000 12.47 ANISOU 1299 C THR 190 1178 1436 2124 -32 -297 - 2321300 O MOTA THR 190 11.959 19.523 50.320 1.000 15.06 ANISOU 1300 O 190 1424 THR 1767 2531 46 -571 -446 MOTA 1301 CB THR 190 9.913 17.297 49.808 1.000 13.16 190 1509 ANISOU 1301 CB THR 1605 1886 -168 80 -121 MOTA 1302 OG1 THR 190 9.481 16.201 48.993 1.000 14.47 ANISOU 1302 OG1 THR 190 1693 1469 2334 -100 -25 -194ATOM 1303 CG2 THR 190 8.778 17.723 50.734 1.000 14.79 ANISOU 1303 CG2 THR 190 1696 1510 2415 73 258 - 89 ATOM 1304 N LEU 191 10.148 20.724 49.732 1.000 12.97 ANISOU 1304 N LEU 191 1329 1449 2149 23 -21 - 286 MOTA 1305 CA LEU 191 10.511 21.908 50.526 1.000 13.75 ANISOU 1305 CA LEU 191 1543 1442 2238 78 -206 -301 ATOM 1306 C LEU 191 9.603 21.964 51.763 1.000 14.47 ANISOU 1306 C . 1689 LEU 191 1543 2265 83 -179 -412 1307 0 LEU 191 8.370 21.868 51.645 1.000 16.58 ANISOU 1307 O LEU 191 1517 219 2486 2297 -176 - 725 ATOM 1308 CB LEU 191 10.398 23.212 49.722 1.000 15.37 ANISOU 1308 CB LEU 191 1717 1444 2680 58 - 106 - 189 1309 CG ATOM LEU 191 11.705 - 23.578 48.973 1.000 16.10 ANISOU 1309 CG 191 1747 LEU 1688 2680 -128 -113 -135 MOTA 1310 CD1 LEU 191 12.069 22.565 47.906 1.000 16.67 ANISOU 1310 CD1 LEU 191 2034 2093 2209 -23 -64 1 9 1311 CD2 LEU 191 11.570 24.959 48.350 1.000 18.53 ANISOU 1311 CD2 LEU 191 2297 1906 2837 -345 -437 1 4 8 ATOM 1312 N 192 10.199 22.148 52.946 1.000 15.36 ILE

- 56 -ANISOU 1312 N ILE 192 1479 2152 2204 -47 -165 - 16422.162 54.194 1.000 15.13 1313 CA ILE 192 9.417 2043 ANISOU 1313 CA ILE 192 1456 2251 -304 -173 -280 ATOM 1314 C ILE 192 9.692 23.423 55.010 1.000 15.58 ANISOU 1314 C ILE 192 1696 1973 2251 -199 -254 -226 192 10.836 23.691 55.381 1.000 17.20 1315 0 MOTA ILE ANISOU 1315 O ILE 192 1856 2449 2229 -307 -341 -574 ATOM 1316 CB ILE 192 9.722 20.920 55.040 1.000 17.03
 192
 2.722
 20.920
 35.040
 1.000
 17.03

 192
 2246
 1958
 2266
 -52
 325

 192
 9.454
 19.596
 54.317
 1.000
 19.80

 192
 3040
 2010
 2473
 -71
 128

 192
 8.995
 20.967
 56.403
 1.000
 18.14

 192
 2278
 2354
 2262
 229
 290

 192
 9.420
 18.387
 55.235
 1.000
 31.57
 ANISOU 1316 CB ILE 325 - 303 1317 CG1 ILE MOTA ANISOU 1317 CG1 ILE 128 - 382 1318 CG2 ILE ANISOU 1318 CG2 ILE 290 -258 1319 CD1 ILE 192 4658 2114 5222 -398 -1094 193 8.625 24.172 55.249 1.000 17.04 ANISOU 1319 CD1 ILE -398 -1094 765 1320 N MOTA GLN ANISOU 1320 M 193 2042 2185 GLN 2248 112 -388 - 301 MOTA 1321 CA 193 8.680 25.291 56.201 1.000 17.70 GLN. ANISOU 1321 CA GLN193 1737 2167 2824 -204 -186 -559 193 7.898 24.869 57.443 1.000 19.67 ATOM 1322 C GLN ANISOU 1322 C GLN 193 1882 2624 2969 -232 211 - 840ATOM 1323 0 GLN 193 7.082 23.942 57.426 1.000 26.60 ANISOU 1323 O GLN 193 2066 3843 4197 -965 -110 6 2 ATOM 1324 · CB 193 8.129 26.598 GLN 55.643 1.000 23.74 193 3070 2388 3561 500 -98 -193 8.913 27.304 54.559 1.000 28.26 ANISOU 1324 CB GLN-98 -514 ATOM 1325 CG GLN ANISOU 1325 CG 193 4664 2384 3689 656 209 0 193 8.338 28.665 54.156 1.000 26.30 GLN MOTA 1326 CD GLN ANISOU 1326 CD 193 2868 2943 193 7.193 28.695 GLN 4181 791 ATOM 1327 OE1 GLN 53.688 1.000 45.31 193 7.193 20.093 193 2826 7147 193 9.080 29.748 193 3609 2588 194 8.241 25.259 194 2926 2758 ANISOU 1327 OE1 GLN 7241 -51 -616 3173 1328 NE2 GLN ATOM 54.345 1.000 30.44 ANISOU 1328 NE2 GLN 5368 413 1259 6 9 2 MOTA 1329 N GLN 58.645 1.000 22.04 ANISOU 1329 N GLN 194 2926 2690 2758 303 -368 - 83 194 7.569 194 3144 1330 CA GLN 24.793 59.847 1.000 22.68 ANISOU 1330 CA GLN2617 2855 82 -230 -150 194 7.275 194 2809 MOTA 1331 C GLN 26.054 60.663 1.000 22.19 ANISOU 1331 C GLN 2768 2856 117 -396 - 320194 7.889 194 4041 ATOM 1332 0 GLN 27.100 60.418 1.000 25.26 ANISOU 1332 O GLN 2877 2679 -313 -21 - 411ATOM 1333 CB 194 8.467 194 4493 23.943 60.739 1.000 29.21 GLNANISOU 1333 CB GLN2707 3899 477 -50 939 1334 CG ATOM GLN 194 9.105 22.735 60.083 1.000 28.80 ANISOU 1334 CG GLN 194 3108 3530 4305 576 -121494MOTA 1335 CD GLN 194 10.296 22.332 60.962 1.000 31.97 ANISOU 1335 CD GLN 194 2961 5384 3800 824 359 1075 1336 OE1 GLN 194 11.421 22.325 60.474 1.000 27.28 ANISOU 1336 OE1 GLN 194 2781 4189 3397 118 133 - 249 1337 NE2 GLN ATOM 194 9.998 22.100 62.232 1.000 29.82 194 3540 3958 3832 989 645 8 195 6.419 25.891 61.658 1.000 23.30 195 2407 3058 3387 -211 -235 -195 6.476 26.833 62.768 1.000 27.14 ANISOU 1337 NE2 GLN 645 800 ATOM 1338 N THR 61.658 1.000 23.30 ANISOU 1338 N THR -211 - 235 - 720ATOM 1339 CA THR ANISOU 1339 CA 195 3459 3544 THR 3308 25 -50 -890 ATOM 1340 C THR 195 6.933 25.997 63.958 1.000 26.11 ANISOU 1340 C THR 195 3825 2829 3268 558 ATOM 1341 0 THR 195 6.639 24.815 63.994 1.000 28.17 ANISOU 1341 O 195 2973 195 5.149 THR 2916 4815 481 171 -1030 ATOM 1342 CB THR 27.534 63.069 1.000 25.87 ANISOU 1342 CB THR 195 3428 2849 3551 -16 -592 -1137

,, ,								101,0250,0000
ATOM	1343	OG1	THR	195	4.111	- 57 - 26 . 550	63 106	1.000 25.45
ANISOU	1343	OG1	THR	195	3427	3101		-9 -117 -750
ATOM			THR		4.788	28.396		1.000 31.31
ANISOU ATOM	1344		PRO		4965 7.604	2552 26.587	4380	
ANISOU	1345	N	PRO		5225	3191	3300	1.000 30.84 785 -517 -1542
MOTA	1346		PRO	196	8.101	25.823	66.065	1.000 28.50
ANISOU ATOM	1346 1347		PRO PRO		3113	3700	4016	-279 -441 -646
ANISOU			PRO		7.018 3581	25.534 3326	67.096 4102	1.000 28.97 42 113 -1381
MOTA	1348	0	PRO	196	6.002	26.229	67.192	1.000 32.32
ANISOU			PRO		4146		3485	901 -180 -1658
ATOM ANISOU	1349	CB	PRO PRO	196	9.094 3888	26.816 3292	66.694 4111	1.000 29.72
ATOM	1350	CG	PRO	196	8.533	28.174	66.364	-285 -353 -1072 1.000 34.87
ANISOU			PRO	196	6285	3575	3390	421 -1326 -1332
ATOM ANISOU	1351		PRO PRO		7.897	28.035	65.012	1.000 33.20
ATOM	1351		CYS		6 407 7.289	3606 24.533	2600 67 919	-598 -494 -1031 1.000 26.96
ANISOU	1352	N	CYS	197	2739	4038	3465	-113 85 -1227
ATOM ANISOU	1353	CA	CYS	197	6.519	24.289	69.126	1.000 31.73
ATOM	1354		CYS CYS	197	3979 6.803	4543 25.412	3533	-39 721 -1726 1.000 35.58
ANISOU	1354	C	CYS	197	4213	4819	4486	-480 1126 -2282
ATOM ANISOU	1355		CYS	197	7.917	25.939	70.175	1.000 31.34
ATOM	1356		CYS CYS		3817 6.940	4845 22.962	3246	36 -383 -992 1.000 35.79
ANISOU	1356	CB	CYS		5913	4705	2980	284 1566 - 1423
ATOM ANISOU	1357		CYS		6.553	21.535		1.000 28.53
ATOM	1358		CYS ALA		3605 5.771	4224 25.791	3009	50 -5 - 4 5 2 1.000 3 7 . 2 7
ANISOU	1358	N	ALA	198	5038	4984	4139	-421 1647 - 2070
ATOM ANISOU	1359		ALA		5.983	26.811	71.888	1.000 35.91
ANISOU	1360		ALA ALA		6273 6.993	4144 26.328	3230	910 522 -1230 1.000 44.30
ANISOU	1360	С	ALA	198	5998	6138	4696	-193 -199 3 3
ATOM	1361	0	ALA	198	7.759	27.127	73.457	1.000 42.85
ANISOU ATOM	1361		ALA ALA	198	5209 4.671	6328 27.231	4742	7 490 - 555
ANISOU	1362	CB	ALA	198	4.671 7588	5697	2557	1.000 41.70 2355 1068 ÷ 721
ATOM	1363		ASN	199	7.036	25.036	73.225	1.000 34.93
ANISOU ATOM	1363	N N	ASN ASN		4027 7.969	5975 24.578	3270	805 167 -621
	1364		ASN		3643	6167	2950	1.000 33.58 -670 -265 -808
ATOM	1365	C	ASN	199	9.352	24.262	73.718	1.000 31.53
ANISOU ATOM	1365		ASN ASN		4077	5048	2853	384 -420 -855
ANISOU	1366	0	ASN		10.153 4223	23.667 5624	74.467 3957	1.000 36.33 -403 -1305 -126
ATOM	1367	СЗ	ASN	199	7.441	23.308		1.000 36.38
ANISOU ATOM	1367 1368		ASN		4533	5029	4262	859 584 - 522
	1368		ASN ASN		7.198 4030	22.180 4863	73.952	1.000 31.28 882 202 178
ATOM	1369	OD1	ASN	199	7.743	22.151		1.000 37.62
ANISOU ATOM	1369 1370	OD1	ASN		4693	6272	3330	122 728 - 56
ANISOU	1370	ND2	ASN		6.393 3508	21.190 6251	74.314	1.000 36.42 -13 1132 - 958
ATOM	1371	N	GLY		9.616	24.569		1.000 30.93
ANISOU ATOM			GLY		4342	4232	3179	436 144 - 692
	1372 1372		GLY GLY		10.920 4430	24.304 4905	71.866 4060	1.000 35.26
ATOM	1373		GLY		11.184	22.886		-317 480 -2400 1.000 36.83

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- 58 -
ANISOU 1373 C
               GLY
                     200 4683
                                4375
                                        4936
                                               -360
                                                     1601 - 1460
       1374 0
               GLY
                     200 12.257
                                22.566 70.897 1.000 32.71
ANISOU 1374 O
               GLY
                     200 3921
                                4072
                                        4436
                                               -377
                                                     752 -1400
ATOM
       1375 N
                PHE
                     201 10.264
                                21.939 71.588 1.000 28.66
ANISOU 1375 N
                PHE
                     201 3813
                                4229
                                        2847
                                               145
                                                     463 - 326
       1376 CA
ATOM
               PHE
                     201 10.491
                                20.575
                                       71.106 1.000 27.55
ANISOU 1376 CA
               PHE
                     201 3190
                                4337
                                        2943
                                               -233
                                                     219 -672
       1377 C
ATOM
                PHE
                     201 10.752
                                20.553 69.600 1.000 24.89
ANISOU 1377 C
                PHE
                     201 2943
                                3682
                                        2832
                                               190
                                                   -268 - 379
ATOM
       1378 0
                                21.255 68.910 1.000 28.22
                PHE
                     201 9.994
ANISOU 1378 O
                PHE
                     201 3583
                                3184
                                        3957
                                               10 -421 277
ATOM
       1379 CB
               PHE
                     201 9.250
                                19.729 71.413 1.000 30.46
ANISOU 1379 CB
               PHE
                     201 3153
                                4862
                                        3560
                                               -371
                                                     -40 - 73
       1380 CG
               PHE
                    201 9.425
                                18.262 71.027 1.000 34.89
ANISOU 1380 CG
               PHE
                    201 4015
                                4609
                                        4632
                                               -772 162 8 9
MOTA
       1381 CD1 PHE
                    201 10.395
                                17.472 71.605 1.000 31.18
ANISOU 1381 CD1 PHE
                    201 3436
                                4103
                                        4310 -875 -93 -1105
ATOM
       1382 CD2 PHE
                    201 8.613
                                17.681
                                        70.078 1.000 28.84
ANISOU 1382 CD2 PHE
                    201 2979
                                        3960
                                4019
                                               329
                                                     612 - 107
       1383 CE1 PHE
MOTA
                    201 10.564 16.160 71.240 1.000 37.73
ANISOU 1383 CE1 PHE
                    201 6489
                                        4239 -1078 -1475 -500
                                3608
ATOM
       1384 CE2 PHE
                    201 8.761
                                16.363 69.679 1.000 31.78
ANISOU 1384 CE2 PHE
                    201 4327
                                3911
                                        3838
                                               652
                                                     250 119
ATOM
       1385 CZ
               PHE
                    201 9.755
                                15.606
                                        70.265 1.000 29.78
ANISOU 1385 CZ
               PHE
                    201 3705
                                3397
                                        4211
                                               6 -638 -849
ATOM
       1386 N
               VAL
                    202 11.706 19.751
                                       69.144 1.000 23.51
ANISOU 1386 N
               VAL
                    202 2671
                                3392
                                        2868
                                               -292
                                                     -1 -578
ATOM
       1387 CA
                    202 11.969 19.626 67.706 1.000 26.37
               VAL
ANISOU 1387 CA
               VAL
                    202 3025
                                        2946
                                4050
                                               -667 57 -724
ATOM
       1388 C
               VAL
                    202 11.423
                               18.283
                                        67.198 1.000 22.75
ANISOU 1388 C
               VAL
                    202 2729
                                3348
                                        2567
                                               96 -120 -435
       1389 0
MOTA
               VAL
                    202 11.880 17.190
                                       67.541 1.000 28.71
ANISOU 1389 O
               VAL
                    202 3249
                                3799
                                        3859
                                               119
                                                     31 6 6 1
       1390 CB
ATOM
               VAL
                    202 13.476
                               19.721
                                        67.415 1.000 24.99
ANISOU 1390 CB
               VAL
                    202 3060
                                3427
                                        3008
                                               -278 283 152
       1391 CG1 VAL
                    202 13.715
                                       65.938 1.000 27.70
                               19.464
ANISOU 1391 CG1 VAL
                    202 4642
                                2577
                                        3307
                                               87 1014 - 3
       1392 CG2 VAL
                    202 14.050
                                21.071
                                       67.823 1.000 26.80
ANISOU 1392 CG2 VAL
                    202 2826
                                3868
                                        3487
                                               -490 474 -398
ATOM
       1393 N
               SER
                    203 10.405
                                18.402
                                       66.333 1.000 24.10
ANISOU 1393 N
               SER
                    203 2194
                                3607
                                        3356
                                               -31
                                                     -179 - 528
ATOM
       1394 CA
               SER
                    203 9.634
                                17.231
                                       65.940 1.000 23.70
ANISOU 1394 CA
               SER
                    203 2373
                                3584
                                        3046
                                               -290 308 -533
       1395 C
MOTA
               SER
                    203 10.168
                                16.511
                                        64.710 1.000 21.28
ANISOU 1395 C
               SER
                    203 2173
                                3041
                                        2871
                                               46 227 - 42
MOTA
       1396 O
                                15.285 64.640 1.000 27.60
               SER
                    203 10.159
ANISOU 1396 O
               SER
                    203 4105
                                3097
                                        3284
                                               -482
                                                     1010 - 249
       1397 CB
               SER
                    203 8.148
                                17.571 65.685 1.000 29.06
ANISOU 1397 CB
               SER
                    203 2251
                                3790
                                        5001
                                               -180
                                                     203 - 2064
ATOM
       1398 OG
               SER
                    203 7.584
                                18.175 66.843 1.000 32.55
ANISOU 1398 OG
               SER
                    203 3840
                                4298
                                        4231
                                               920
                                                     1099 - 382
MOTA
       1399 N
               LEU
                    204 10.688
                                17.233
                                        63.724 1.000 22.46
ANISOU 1399 N
               LEU
                    204 2476
                                3013
                                        3043
                                               79 450 - 46
ATOM
       1400 CA
               LEU
                    204 11.166
                                16.530 62.544 1.000 20.26
ANISOU 1400 CA
               LEU
                    204 2200
                                2831
                                        2667
                                               45 -18 - 15
ATOM
       1401 C
               LEU
                    204 12.595
                                16.038
                                        62.747 1.000 18.83
ANISOU 1401 C
               LEU
                    204 2151
                                        2477
                                2528
                                               -75
                                                     60 - 1
ATOM
       1402 0
                    204 13.443
               LEU
                                        63.251 1.000 20.47
                                16.783
ANISOU 1402 O
               LEU
                    204 2333
                                2386
                                        3059
                                              -303
                                                     -195 4 0 4
ATOM
       1403 CB
               LEU
                    204 11.103
                                17.486
                                        61.362 1.000 21.42
ANISOU 1403 CB
               LEU
                    204 2718
                                2548
                                        2871
                                               311
                                                     -16
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- 59 -1404 CG LEU 204 9.769 18.188 61.079 1.000 33.57 MOTA 1404 CG LEU 204 2820 4319 5617 177 -1316 117 1405 CD1 LEU 204 9.797 18.747 59.660 1.000 36.19 1406 CD2 LEU 204 8.581 17.234 61.219 1.000 37.76 1406 CD2 LEU 204 3058 5328 5860 ANISOU 1404 CG LEU 204 2820 -1316 1172 ANISOU 1405 CD1 LEU ANISOU 1406 CD2 LEU 204 3058 5328 5960 -526 -1896 205 12.864 14.836 62.284 1.000 20.33 -526 -1896 686 1407 N GLN ANISOU 1407 N GLN 1408 CA GLN 205 2522 2225 2425 -6 -181 3 6 205 14.512 13.504 61.036 1.000 18.19 ANISOU 1408 CA GLN MOTA1409 C GLN 205 14.512 13.504 51.035 1.000 15.19 205 1986 2383 2543 -143 -188 -1 205 13.577 13.033 60.408 1.000 19.87 205 1974 3063 2514 -125 -212 -2 205 14.296 13.267 63.493 1.000 24.25 205 3948 2716 2548 202 -343 2 ANISOU 1409 C GLN -188 - 801410 O GLN ATOM ANISOU 1410 O GLN -125 -212 -237 1411 CB GLN ATOM ANISOU 1411 CB GLN -343 2 9 6 205 14.164 13.948 64.856 1.000 30.64 205 4099 5159 2382 850 -327 -1412 CG GLN ATOM ANISOU 1412 CG GLN -327 - 89ATOM 1413 CD GLN 205 14.744 13.078 65.948 1.000 28.28 ANISOU 1413 CD GLN 205 4473 3633 2640 -161 -1015 -1015 - 390ATOM 1414 OE1 GLN 205 14.307 11.921 66.041 1.000 37.69 ANISOU 1414 OE1 GLN 205 5733 5073 3515 -2145 -699 4 7 8 ANISOU 1425 CB GLU 207 3401 1784 3946 316 -1226 6 1 ATOM 1426 CG GLU 207 19.757 7.674 58.295 1.000 24.35 ANISCU 1426 CG GLU 207 3223 1907 4121 354 93 467 ATOM 1427 CD GLU 207 20.730 7.791 57.129 1.000 31.69 ANISOU 1427 CD GLU 207 2729 5178 4134 -1218 -175 1 2 2

ATOM 1428 OE1 GLU 207 20.376 7.611 55.943 1.000 26.97

ANISOU 1428 OE1 GLU 207 2849 3404 3993 31 -256 3 0 9

ATOM 1429 OE2 GLU 207 21.908 8.121 57.407 1.000 3 0.70

ANISOU 1429 OE2 GLU 207 2484 3416 5764 -233 -342 -1168

ATOM 1430 N VAI 208 20 219 10 236 50 078 1.000 1 8 52 ATOM 1430 N VAL 208 20.919 10.936 59.078 1.000 18.53 ANISOU 1430 N VAL 208 2020 2112 2907 130 -362 3 2 0 ATOM 1431 CA VAL 208 22.150 11.547 58.541 1.000 19.53 ANISOU 1431 CA VAL 208 2044 2238 3137 39 -476 6 3 0 ATOM 1432 C VAL 208 23 341 10.755 ATOM 1432 C 208 23.341 10.755 59.088 1.000 21.95 VAL ANISOU 1432 C VAL 208 2040 2792 3507 225 -461 7 ATOM 1433 O VAL 208 23.460 10.663 60.314 1.000 23.82 ANISOU 1433 O VAL 208 2262 3240 3547 -40 -858 8 ATOM 1434 CB VAL 208 22.271 13.027 58.905 1.000 19.72 3507 225 -461 797 3547 -40 -858 8 2 5

ANTCOL	1 1 2 1	CD	173.1	200	1010	- 60 -	5.5.4.5		
ANISOU ATOM	1434				1918 23.524	2429	3145		-308 3 1 1
ANISOU					25.524	13.626 2374	3895	-202	23.14 284 349
ATOM	1436				21.030	13.812	58.469		
ANISOU					2462	2279	2658	232	-667 - 87
ATOM	1437		GLY		24.180	10.169	58.246		
ANISOU			GLY		2500	2449	4123	465	-711 3 6
ATOM	1438	CA	GLY		25.306	9.374	58.773		
ANISOU			GLY		1987	3599 `	4450 .	460	-487 5 1 6
ATOM	1439		GLY		24.905	8.250	59.695		30.01
ANISOU			GLY		3469	3240	4693	238	-1422 732
ATOM	1440		GLY		25.609	7.835	60.629		
ANISOU ATOM	1440		GLY GLY		4053	4458	3438	1225	-897 8 3
ANISOU			GLY	210	23.691 3165	7.702 3214	59.523 3744		
ATOM	1442		GLY		23.263	6.585	60.360	259	-86 350 29.78
ANISOU			GLY		4603	3091	3619	-55	-997 5 8 4
ATOM	1443		GLY		22.622	6.993	61.663		
ANISOU	1443	С	GLY		5827	4212	4507	-2536	732 5 0
MOTA	1444		GLY		22.160	6.187	62.481		
ANISOU			GLY		4152	6516	5082	-1874	-567 2346
ATOM	1445		ALA		22.512	8.274	61.976	1.000	
ANISOU ATOM	1445		ALA ALA		4803 21.828	4625	3037		-1177 632
ANISOU			ALA		3993	8.603 5958	63.235 3584		
ATOM	1447		ALA		20.663	9.543	62.940	1061	-610 9 7 0 ·
ANISOU			ALA		3508	4737			69 1854
MOTA	1448		ALA	211	20.652	10.097			
ANISOU			ALA	211	3661	4062	3020	-571	-551 1010
ATOM	1449		ALA		22.812	9.278	64.170		41.36
ANISOU			ALA		3644	8904	3169		-18 -791
ATOM ANISOU	1450		PHE PHE		19.682 5211	9.676	63.825		
ATOM	1451		PHE		18.620	4237 10.654	4489 63.641	1166	1265 2171
ANISOU			PHE		4490	3167	3293	263	504 1037
ATOM	1452		PHE		19.100	12.023	64.124		
ANISOU			PHE		6746	3760	2685	-248	-539 776
ATOM	1453		PHE		19.667	12.191			
ANISOU			PHE		6144	5384			-1129 1220
ATOM	1454		PHE		17.358	10.219	64.388		
ANISOU ATOM			PHE		6376	2569	0200	1348	3748 2314
ANISOU			THR THR		18.906 4134	13.008			26.30
ATOM	1456		THR		19.424	2738 14.359	3122	662	-581 1 0 0 25.08
ANISOU			THR		3587	2852	3089	767	-810 - 323
ATOM	1457	С	THR	213		15.283	63.400		
ANISOU			THR		2835	2652	3560	215	-855 -643
ATOM	1458		THR		17.329	15.137			21.40
ANISOU			THR		2640	2269	3223	-328	-580 -179
ATOM ANISOU	1459		THR THR		20.398	14.759			27.60
ATOM	1460				3155 21.673	3220	4113	189	-356 - 798
ANISOU					3582	14.084 4220	4356	746	32.00 -410 520
ATOM	1461				20.735	16.254			29.45
ANISOU	1461	CG2	THR		4422	3320	3448	-106	-1265 - 204
MOTA	1462	N	ASP	214	18.119	16.177			21.05
ANISOU			ASP	214	2790	2236	2972	-82	-380 -142
ATOM	1463		ASP		17.001	17.110	64.462		20.61
ANISOU			ASP		2742	2095	2993	-117	-898 - 379
ATOM ANISOU	1464		ASP ASP		16.994	18.030			20.58
FT4 + 200	T 4 Q 4		ASP	214	2373	2525	2923	182	-169 -237

1465 C ASP 214 18.018 18.430 62.678 1.000 23.02 ATOM 214 2461 2883 3404 -167 -52 -5 214 17.205 18.058 65.637 1.000 23.54 214 3304 2607 3032 -92 -748 -6 ANISOU 1465 O ASP -167 -52 -572 1456 CB ASP ANISOU 1466 CB ASP -92 -748 -668 MOTA 1467 CG ASP 214 16.915 17.506 67.004 1.000 24.93 ANISOU 1467 CG ASP 214 3545 2850 3079 450 -417 -614 1468 OD1 ASP MOTA 214 16.357 16.395 67.113 1.000 29.17 ANISOU 1468 OD1 ASP 214 4134 3070 3878 202 -705 2 6 2 1469 OD2 ASP 214 17.276 18.191 67.990 1.000 34.38 MOTA ANISOU 1469 OD2 ASP 214 6917 3040 3107 1017 -1413 - 736 1470 N MOTA LEU 215 15.802 18.452 62.859 1.000 20.74 ANISOU 1470 N 215 2426 2372 3081 86 -60 3 0 6 215 15.568 19.401 61.796 1.000 20.55 LEU MOTA 1471 CA LEU 215 2895 2013 2899 -202 -176 1 215 14.724 20.552 62.332 1.000 19.02 ANISOU 1471 CA LEU -202 -178 1 4 1 1472 C ATOM LEU 215 2482 2240 2504 -142 -34 3 215 13.510 20.613 62.142 1.000 22.39 ANISOU 1472 C LEU -142 -34 321 1473 0 MOTA LEU 215 2635 2483 3389 -160 -475 5 215 14.826 18.722 60.650 1.000 22.04 ANISOU 1473 O LEU -160 -475 5 7 3 1474 CB LEU 215 2778 ANISOU 1474 CB LEU 2510 3086 -140 -261 - 65 1475 CG 215 15.598 17.502 60.128 1.000 25.25.25.215 3680 2829 2005 LEU ANISOU 1475 CG LEU 215 3680 2829 3085 85 - 166 - 402 ATOM 1476 CD1 LEU 215 14.680 16.736 59.174 1.000 27.12 ANISOU 1476 CD1 LEU 215 4886 2934 2482 419 -1128 - 65 1477 CD2 LEU ATOM 215 16.881 18.046 59.510 1.000 30.76 ANISOU 1477 CD2 LEU 215 3434 3089 5165 1003 524 1478 N ATOM PRO 216 15.383 21.433 63.078 1.000 19.68 ANISOU 1478 N PRO 216 2407 2191 2879 -157 148 103 ATOM 1479 CA PRO 216 14.665 22.534 63.708 1.000 22.42 ANISOU 1479 CA PRO 216 2869 2812 2836 272 10 - 228 MOTA 1480 C PRO 216 14.201 23.576 62.698 1.000 25.36 ANISOU 1480 C PRO 216 4118 2433 3086 566 -131 - 3 1 5 ATOM 1481 0 216 14.700 23.759 61.586 1.000 24.67 PRO ANISOU 1481 O PRO 216 3682 2406 3284 187 -176 - 26 216 15.693 23.092 64.676 1.000 23.88
216 3108 3049 2917 -216 116 -318
216 17.033 22.701 64.146 1.000 28.31
216 2994 2996 4766 -88 -117 -1454
216 16.807 21.405 63.436 1.000 24.55
216 2353 1777 5197 -436 -83 -348
217 13.154 24.287 63.102 1.000 24.13
217 3237 2704 3229 244 -631 -511
217 12.676 25.510 62.462 1.000 26.08
217 2514 2899 4498 104 -592 3 9
217 13.824 26.516 62.369 1.000 25.24
217 3049 2948 3592 -257 -506 -5 38
217 14.570 26.675 63.340 1.000 31.78
217 4114 2863 5096 -352 -2151 5 6 4
217 11.559 26.103 63.315 1.000 25.97.
217 2747 2773 4346 86 -615 -167
217 11.189 27.543 63.125 1.000 31.64
217 3080 2803 6139 338 -1473 - 6 4 4
217 10.430 27.928 62.022 1.000 27.85
217 2238 3029 5314 511 -175 9 3 ATOM 1482 CB PRO 216 15.693 23.092 64.676 1.000 23.88 ANISOU 1482 CB PRO 1483 CG ATOM PRO ANISOU 1483 CG PRO MOTA 1484 CD PRO ANISOU 1484 CD PRO ATOM 1485 N TYR ANISOU 1485 N TYR 1486 CA TYR ANISOU 1486 CA \mathtt{TYR} 1487 C TYR ANISOU 1487 C TYR ATOM 1488 0 TYR ANISOU 1488 O TYRATOM 1489 CB TYR ANISOU 1489 CB TYR ATOM 1490 CG TYR ANISOU 1490 CG TYR ATOM 1491 CD1 TYR ANISOU 1491 CD1 TYR 217 2238 3029 5314 511 -175 9 3 217 11.512 28.522 64.069 1.000 38.49 1492 CD2 TYR MOTA ANISOU 1492 CD2 TYR 217 4721 2813 7093 -686 -1682 -749 1493 CE1 TYR 217 10.021 29.219 61.772 1.000 26.53 ANISOU 1493 CE1 TYR 217 1908 2675 5496 -41 107 6 9 ATOM 1494 CE2 TYR 217 11.113 29.835 63.827 1.000 42.90 ANISOU 1494 CE2 TYR 217 7112 2347 6842 -1415 -1949 - 218 1495 CZ \mathtt{TYR} 217 10.373 30.168 62.712 1.000 34.93

- 62 -ANISOU 1495 CZ TYR 217 4042 2747 6483 -1462 -545 1 6 6 1496 OH TYR 217 9.996 31.486 62.473 1.000 36.41 ANISOU 1496 OH TYR 217 5499 2895 5439 -753 -250 -289 ATOM 1497 N ARG 218 14.022 27.110 61.218 1.000 25.58 218 3461 2406 3852 227 ANISOU 1497 N ARG 218 3461 2406 -227 1498 CA ARG 218 14.923 28.243 61.049 1.000 29.26 1498 CA ARG 218 3630 3270 4219 -784 -1349 3852 -533 - 476 ANISOU 1498 CA ARG 218 3630 -1349 268 1499 C ARG 218 14.113 29.336 60.366 1.000 24.81 ANISOU 1499 C ARG 218 4063 2949 2415 -382 -228 - 56 ARG 218 13.746 29.174 59.212 1.000 29.56 ATOM 1500 0 ANISOU 1500 O ARG 218 6298 2267 2666 -890 -994 1 6 5 ATOM 1501 CB ARG 218 16.162 27.823 60.256 1.000 35.90 218 3223 3685 6732 -624 -703 8 ANISOU 1501 CB ARG 3685 6732 -624 -703 8 9 6 218 17.369 28.665 60.661 1.000 51.38 1502 CG ATOM ARG ANISOU 1502 CG 218 4740 6768 8015 -3031 430 -183 218 18.539 28.606 59.701 1.000 38.84 ARG MOTA 1503 CD ARG 218 4968 6308 3482 -3596 -1165 164 218 19.343 27.395 59.905 1.000 45.09 218 4655 7495 4982 -2325 -962 - 94 218 20.272 27.208 58.959 1.000 55.53 ANISOU 1503 CD ARG -3596 -1165 1647 1504 NE ATOM ARG ANISOU 1504 NE ARG 1505 CZ ATOM ARG 218 20.272 27.208 58.959 1.000 55.53 218 5299 11458 4340 -2701 -1188 -1948 218 20.289 28.158 58.031 1.000 60.85 218 2399 16648 4071 -1943 -1333 548 218 21.060 26.165 59.001 1.000 60.37 218 8580 10111 4247 -2152 639 -4241 219 13.871 30.496 60.972 1.000 25.89 219 2625 4126 3086 35 296 -1014 219 13.065 31.548 60.326 1.000 28.10 219 2828 3120 4730 -410 379 -696 219 13.636 31.959 58.981 1.000 28.43 219 3141 3010 4653 -190 116 -328 219 12.904 32.393 58.081 1.000 34.17 ANISOU 1505 CZ ARG MOTA 1506 NH1 ARG ANISOU 1506 NH1 ARG ATOM 1507 NH2 ARG ANISOU 1507 NH2 ARG ATOM 1508 N PRO ANISOU 1508 N PRO MOTA 1509 CA PRO ANISOU 1509 CA PRO ATOM 1510 C PRO ANISOU 1510 C PRO ATOM 1511 0 PRO 219 12.904 32.393 58.081 1.000 34.17 ANISOU 1511 O PRO 219 4734 3500 4750 302 -798 - 893ATOM 1512 CB PRO 219 13.115 32.717 61.316 1.000 39.70 ANISOU 1512 CB PRO 219 5621 3612 5852 -500 1615 -1527 ATOM 1513 CG 219 13.368 32.033 62.628 1.000 42.38 PRO ANISOU 1513 CG PRO 219 6139 5277 4688 -257 2084 -2086 ATOM 1514 CD 219 14.370 30.943 62.289 1.000 32.77 PRO ANISOU 1514 CD PRO 219 3901 5719 2831 -602 828 -1603 ATOM 1515 N 220 14.950 31.824 58.811 1.000 25.65 ASP ANISOU 1515 N ASP 220 3328 1582 4837 -276 801 -878 1516 CA ASP ATOM 220 15.590 32.280 57.587 1.000 26.45 220 3594 2115 4341 -782 248 -8 ANISOU 1516 CA ASP 2115 4341 -782 248 -861 ATOM 1517 C 220 15.781 31.305 56.451 1.000 28.46 ASP ANISOU 1517 C ASP 220 3549 1843 5423 -111 1638 - 943 220 16.432 31.620 55.433 1.000 25.80 MOTA 1518 O ASP. ANISOU 1518 O ASP 220 3249 2021 4533 -140 623 -412 MOTA 1519 CB ASP 220 16.911 32.962 57.998 1.000 33.76 ANISOU 1519 CB ASP 220 2351 6938 -445 1187 -1724 3539 1520 CG ATOM 220 17.882 31.913 58.502 1.000 42.36 ASP ANISOU 1520 CG ASP 220 2653 3531 9912 -812 230 -957 1521 OD1 ASP 220 17.484 31.170 59.423 1.000 37.00 ANISOU 1521 OD1 ASP 220 3154 4148 6757 -104 -410 -2001 1522 OD2 ASP 220 18.981 31.787 57.957 1.000 37.34 ANISOU 1522 OD2 ASP 220 2520 4700 6969 93 -824 -1266 ATOM 1523 N ALA 221 15.292 30.072 56.537 1.000 24.79 ANISOU 1523 N ALA221 4148 1872 3398 -252 671 -659 ATOM 1524 CA ALA 221 15.695 29.016 55.596 1.000 19.17 ANISOU 1524 CA ALA 221 2165 1868 3251 -52 -92 -610 ATOM 1525 C ALA 221 14.551 27.996 55.479 1.000 18.60 ANISOU 1525 C ALA221 1920 2238 2908 -82 -207 - 362

- 63 -ATOM 1526 0 ALA 221 13.763 27.852 56.415 1.000 26.47 1526 O ALA 221 4127 2641 3289 -1307 894 -1527 CB ALA 221 16.939 28.316 56.104 1.000 19.36 ANISOU 1526 O 2641 3289 -1307 894 -904 ANISOU 1527 CB ALA 221 2054 2333 2969 -537 -316 6 6 1528 N VAL 222 14.490 27.385 54.313 1.000 17.35 ANISOU 1528 N VAL 222 2089 1841 2661 -101 -323 - 154 MOTA 1529 CA VAL 222 13.556 26.276 54.083 1.000 17.45 ANISOU 1529 CA VAL 222 1620 2004 3004 -66 MOTA 1530 C VAL 222 14.333 24.965 54.077 1.000 15.69

 222
 14.333
 24.965
 54.077
 1.000
 15.69

 222
 1616
 1876
 2471
 -269
 -349 - 324

 222
 15.512
 24.934
 53.716
 1.000
 17.84

 222
 1658
 1730
 3390
 -108
 -1944
 8

 222
 12.822
 26.433
 52.747
 1.000
 19.60

 222
 2267
 2202
 2979
 91
 -666
 -304

 222
 13.781
 26.363
 51.563
 1.000
 21.96

 222
 2252
 3113
 2977
 250
 -645 - 182

 222
 11.730
 25.411
 52.490
 1.000
 22.44

 222
 2923
 2537
 3067
 -497
 -898
 4

 ANISOU 1530 C VAL 1531 0 ATOM VAL ANISOU 1531 O VAL 1532 CB MOTA VAL ANISOU 1532 CB VAL ATOM 1533 CG1 VAL ANISOU 1533 CG1 VAL 1534 CG2 VAL ATOM 222 2923 2537 3067 -497 -898 4 4 223 13.789 23.892 54.621 1.000 16.30 ANISOU 1534 CG2 VAL 1535 N LEU 223 1792 1694 2706 -239 -93 -532 223 14.407 22.575 54.579 1.000 15.91 223 1679 1864 2503 -93 -297 -333 223 14.114 21.908 53.243 1.000 14.86 ANISOU 1535 N LEU MOTA 1536 CA LEU ANISOU 1536 CA LEU 1537 C MOTA LEU ANISOU 1537 C LEU 223 1337 1537 2773 -141 -322 - 458 223 12.969 21.888 52.766 1.000 16.23 ATOM 1538 O LEU ANISOU 1538 O LEU 223 1317 2132 2719 70 -391 -281 ATOM 1539 CB LEU 223 13.829 21.779 55.761 1.000 19.97 ANISOU 1539 CB LEU 223:2740 1945 2901 -121 205 -212 ATOM 1540 CG LEU 223 14.298 20.348 55.882 1.000 23.01 ANISOU 1540 CG 1540 CG LEU 223 2658 1871 4205 -375 -170 9 1541 CD1 LEU 223 15.797 20.322 56.143 1.000 23.73 -375 -170 9 1 ANISOU 1541 CD1 LEU 223 2570 3067 3378 69 135 3 1 6 1542 CD2 LEU 223 13.492 19.668 56.979 1.000 35.71 ANISOU 1542 CD2 LEU 223 2813 3296 7459 525 1116 2333 1543 N ATOM VAL 224 15.115 21.370 52.570 1.000 14.18 ANISOU 1543 N VAL -320 - 2051544 CA VAL MOTA ANISOU 1544 CA VAL 224 1585 1501 2431 -23 -323 -224 15.320 19.160 51.561 1.000 13.59 -323 -127 ATOM 1545 C VAL ANISOU 1545 C 224 1464 1522 2178 23 -290 -25 224 16.442 18.861 51.981 1.000 15.38 VAL 23 -290 -251 ATOM 1546 O VAL ANISOU 1546 O 224 1464 1558 2822 0 -505 -37 224 15.832 21.209 50.222 1.000 14.25 VAL 0 -505 -374 1547 CB VAL MOTA ANISOU 1547 CB VAL 224 1402 1606 2407 -60 -461 -108 224 15.685 20.443 48.906 1.000 16.63 1548 CG1 VAL ANISOU 1548 CG1 VAL 224 1682 2164 2474 -159 -408 - 421 1549 CG2 VAL 224 15.575 22.687 50.040 1.000 16.40 ANISOU 1549 CG2 VAL 224 1807 2863 6 ~509 8 7 1562 ATOM 1550 N 225 14.340 18.299 51.299 1.000 13.49 PHE ANISOU 1550 N PHE 225 1494 1526 2106 -66 -353 - 130 MOTA 1551 CA PHE 225 14.647 16.882 51.162 1.000 14.67 ANISOU 1551 CA PHE 225 1639 -61 -283 1505 2431 -115 MOTA 1552 C PHE 225 14.756 16.533 49.675 1.000 14.27 ANISOU 1552 C PHE 225 1536 2352 -260 - 194 1533 100 1553 O ATOM PHE 225 13.858 16.876 48.893 1.000 16.25 ANISOU 1553 O PHE 225 1604 2000 2569 296 -311 - 88 1554 CB PHE 225 13.537 15.999 51.749 1.000 15.57 ANISOU 1554 CB PHE 225 1613 1563 2740 -25 -46 2 4 ATOM 1555 CG PHE 225 13.387 15.996 53.257 1.000 17.95 ANISOU 1555 CG PHE 225 1888 2267 2666 -650 -302 2 0 3 1556 CD1 PHE 225 14.409 15.809 54.157 1.000 27.39

- 64 -

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ANISOU 1556 CD1 PHE
                    225 2740
                                4234
                                        3431
                                             -910 -1094 900
       1557 CD2 PHE
                    225 12.125
                                15.863 53.820 1.000 21.09
ANISOU 1557 CD2 PHE
                    225 2333
                                2765
                                        2917
                                               -166 399 -527
       1558 CE1 PHE
MOTA
                    225 14.211
                                15.673
                                        55.521 1.000 26.82
ANISOU 1558 CE1 PHE
                    225 3108
                                        3424 -1044 -1241 1128
                                3657
       1559 CE2 PHE
ATOM
                    225 11.910
                                15.910
                                        55.186 1.000 21.65
ANISOU 1559 CE2 PHE
                    225 2994
                                2414
                                        2817 623
                                                     239 - 39
ATOM
       1560 CZ
               PHE
                    225 12.958
                                15.787
                                        56.078 1.000 28.82
ANISOU 1560 CZ
               PHE
                    225 3705
                                3716
                                        3531
                                               -832 -663 3 4 0
MOTA
       1561 N
                CYS
                                       49.266 1.000 12.77
                    226 15.795
                                15.817
ANISOU 1561 N
                CYS
                    226 1428
                                1292
                                               -60 -370 -239
                                        2131
MOTA
       1562 CA
                    226 15.810 15.180 47.956 1.000 12.99
               CYS
ANISOU 1562 CA
               CYS
                    226 1360
                                1440
                                        2135
                                               12 -355 - 207
MOTA
       1563 C
               CYS
                    226 14.903 13.956 47.985 1.000 12.37
ANISOU 1563 C
               CYS
                    226 1533
                    226 1533 1212 1955 8 -283 -311
226 14.961 13.217 48.974 1.000 15.68
                                1212
                                        1955
ATOM
       1564 0
               CYS
ANISOU 1564 O
               CYS
                    226 1885
                                1651
                                        2424
                                               -140 -611 158
       1565 CB
               CYS
                    226 17.228 14.855 47.527 1.000 13.77
ANISOU 1565 CB
               CYS
                    226 1410
                                1627
                                        2193
                                               19 -203 - 75
ATOM
       1566 SG
               CYS
                    226 18.224 16.367
                                       47.314 1.000 16.37
ANISOU 1566 SG
               CYS
                    226 1744
                                        2735
                                1740
                                               -222 -236 -12
ATOM
       1567 N
               GLY
                    227 14.150 13.722
                                       46.928 1.000 13.20
ANISOU 1567 N
               GLY
                    227 1388
                                1513
                                        2113
                                               -28
                                                     -293 - 290
ATOM
       1568 CA
               GLY
                    227 13.352 12.496
                                       46.899 1.000 12.58
ANISOU 1568 CA
               \mathsf{GLY}
                    227 1279
                                1631
                                        1872
                                               -83
                                                     -438 - 255
ATOM
       1569 C
               GLY
                    227 13.903 11.541
                                        45.849 1.000 12.54
ANISOU 1569 C
               GLY
                    227 1518
                                1279
                                        1965
                                               15 - 288 - 79
ATOM
       1570 O
               GLY
                    227 14.917
                               11.732
                                       45.152 1.000 13.58
ANISOU 1570 O
               GLY
                    227 1630
                                1523
                                        2008
                                               51 -155 8 2
ATOM
       1571 N
               ALA
                    228 13.212
                                10.400
                                        45.712 1.000 13.02
ANISOU 1571 N
               ALA
                    228 1490
                                1306
                                        2151 59 -204 -161
44.860 1.000 12.41
      1572 CA ALA
ATOM
                    228 13.663
                                9.321
ANISOU 1572 CA ALA
                    228 1649
                                1155
                                        1912
                                               -68
                                                   -119 - 63
ATOM
       1573 C
               ALA
                    228 13.706
                                9.727
                                        43.404 1.000 12.82
ANISOU 1573 C
               ALA
                    228 1566
                                1288
                                        2016
                                               97 -223 - 5
ATOM
      1574 O
               ALA
                    228 14.482
                                9.132
                                        42.651 1.000 13.64
ANISOU 1574 O
               ALA
                    228 1717
                                1462
                                        2004
                                               26 -6 -131
ATOM
       1575 CB
               ALA
                    228 12.714 8.121
                                        45.058 1.000 14.56
ANISOU 1575 CB
               ALA
                    228 1808
                                1366
                                        2356
                                               -219
                                                     358 - 243
ATOM
       1576 N
                    229 12.909 10.695
               ILE
                                       42.952 1.000 13.61
ANISOU 1576 N
               ILE
                    229 1340
                                1391
                                        2441
                                               -43
                                                     -289 273
ATOM
       1577 CA
               ILE
                    229 13.024 11.131
                                       41.566 1.000 12.93
ANISOU 1577 CA
               ILE
                    229 1325
                                1243
                                        2344
                                               -42
                                                     -306 1 7 3
MOTA
       1578 C
               ILE
                    229 14.342 11.864
                                       41.358 1.000 13.17
ANISOU 1578 C
               ILE
                    229 1327
                                1364
                                        2311
                                               -47
                                                     -191 1 3 0
ATOM
       1579 O
               ILE
                    229 14.938 11.746
                                       40.262 1.000 14.41
ANISOU 1579 O
               ILE
                    229 1587
                                                   -167 183
                                1596
                                        2293
                                               -37
ATOM
      1580 CB
               ILE
                    229 11.768 11.888
                                       41.103 1.000 13.46
ANISOU 1580 CB
               ILE
                    229 1470
                                1631
                                        2015
                                               171
                                                     -354 - 42
ATOM
       1581 CG1 ILE
                    229 10.599 10.920
                                       40.973 1.000 15.72
ANISOU 1581 CG1 ILE
                    229 1218
                                1936
                                        2817
                                               85 31 1 1 8
ATOM
      1582 CG2 ILE
                    229 12.040 12.674 39.808 1.000 14.19
ANISOU 1582 CG2 ILE
                    229 1670
                                1425
                                        2298
                                               76 -364 174
       1583 CD1 ILE
                    229 10.745 9.924
                                        39.836 1.000 20.03
ANISOU 1583 CD1 ILE
                    229 2129
                                1814
                                        3667
                                               -208 -385 -488
       1584 N
               ALA
                    230 14.877 12.575 42.353 1.000 13.38
ANISOU 1584 N
               ALA
                    230 1252
                                1378
                                        2454
                                               -97
       1585 CA ALA
                    230 16.209 13.185 42.130 1.000 12.30
ANISOU 1585 CA ALA
                    230 1156
                                1444
                                        2074
                                               66 -97 -108
       1586 C
               ALA
                    230 17.223 12.033 41.976 1.000 12.89
ANISOU 1586 C
               ALA
                    230 1491
                                1327
                                        2079
                                               128
                                                     30 - 20
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						1 6 17 6 12 6 7 6 5 6 6 6
ATOM	1587 0	ALA	230 18.100	-65- 12.091	41 146	1.000 13.65
	J 1587 O	ALA	230 1240	1530	2418	108 4 4 6
ATOM	1588 CB	ALA	230 16.588	14.000	43.345	1.000 13.66
ANISOC	J 1588 CB 1589 N	$_{ m ALA}$	230 1559		2215	-186 -21 -229
	J 1589 N	THR	231 17.143 231 1526	10.978 1318	42.805 2214	1.000 13.31
ATOM	1590 CA	THR	231 18.022	9.815	42.659	58 -261 - 1 1.000 13.32
	J 1590 CA	THR	231 1660	1307	2093	78 -302 3 2
ATOM	1591 C J 1591 C	THR	231 17.906	9.224	41.251	1.000 13.27
ATOM	1592 0	THR	231 1300 231 18.932	1631 8.974	2111	205 -211 3
ANISOU	1592 0	THR	231 1468	1759	2667	1.000 15.51 245 58 - 170
ATOM	1593 CB	THR	231 17.656	8.751	43.688	1.000 13.03
ANISOU	1593 CB 1594 OG3	THR	231 1500	1302	2151	46 -166 1 2
	1594 OG1	THR	231 17.530 231 1742	9.313 1614	44.995	1.000 14.70
ATOM	1595 CG2	THR	231 18.698	7.621	2230 43 697	-99 32 - 14 1.000 13.69
	1595 CG2		231 1449	1419	2335	113 -211 1 9 7
ATOM	1596 N 1596 N	LEU	232 16.665	9.049	40.796	1.000 13.43
ATOM	1597 CA	LEU LEU	232 1447 232 16.446	1384 8.396	2271	75 -404 - 27
ANISOU	1597 CA	LEU	232 1809	1226	2326	1.000 14.11 80 -468 4 9
ATOM	1598 C	LEU	232 16.975	9.248		1.000 15.53
ANISOU	1598 C 1599 O	LEU	232 1968	1557	2376	209 -3 9 0
	1599 0	LEU LEU	232 17.749 232 2024	8.808 1949	37.504 2546	1.000 17.16
ATOM	1600 CB	LEU	232 14.940	8.135		107 -116 - 519 1.000 14.47
ANISOU		LEU	232 1692	1630	2175	72 -396 -161
ATOM ANTSOU	1601 CG 1601 CG	LEU LEU	232 14.525 232 1941	7.307	38.155	1.000 15.89
ATOM	1602 CD1	LEU	232 1941 232 15.118	1768 5.920	2329 38.202	120 -470 - 303
ANISOU	1602 CD1	LEU	232 3565	2020	3228	1.000 23.19 743 -1110 -851
ATOM	1603 CD2	LEU	232 13.003		38.126	1.000 19.46
ATOM	1603 CD2 1604 N	VAL	232 2006 233 16.539	2262	3126	-470 -523 - 66
	1604 N	VAL	233 16.539	10.514 1454	38.299	1.000 13.73 -7 -263 193
ATOM	1605 CA		233 16.893	11.317		1.000 13.84
ANISOU ATOM	1605 CA 1606 C	VAL	233 1674	1658	1926	141 -73 107
ANISOU		VAL VAL	233 18.407 233 1716	11.510	37.025	1.000 14.08
ATOM	1607 O	VAL	233 18 940	1674 11.587	1958	72 - 46 1 1 3 1.000 16.65
ANISOU	1607 0	VAL	233 1923	2325	2079	38 109 4 0 1
ATOM	1608 CB 1608 CB		233 16.098	12.626	37.062	1.000 14.69
ATOM	1609 CG1	VAL VAL	233 1680 233 16.529	1696	2206	141 -165 3 3 3
ANISOU	1609 CG1	VAL	233 1615	13.650 1654	2698	1.000 15.70 34 156 - 28
ATOM	1610 CG2	VAL	233 16.117	13.206		1.000 16.43
ANISOU	1610 CG2 1611 N		233 1740	2041	2459	251 117 596
ANISOU	1611 N	\mathtt{THR}	234 19.100 234 1599	11.594 1724	38.175 2083	1.000 14.23
ATOM	1612 CA	THR	234 20.524	11.908		146 -110 2 3 5 1.000 16.14
	1612 CA	THR	234 1664	1868	2602	63 -171 - 49
ATOM ANISOU	1613 C	THR	234 21.346	10.621		1.000 17.09
ATOM	1614 0	THR	234 1717 234 22.558	1865 10.644	2912	146 211 - 51
ANISOU	1614 0	THR	234 1776	1951	2828	1.000 17.25 108 200 229
ATOM	1615 CB	THR	234 21.030	12.681		1.000 15.29
ANISOU	1615 CB 1616 OG1	THR	234 1667	1502	2642	-46 -149 1 6 3
	1616 OG1	THR	234 20.849 234 1659	11.819 1708		1.000 15.45
ATOM	1617 CG2	THR	234 1039	1708	2502 39.597	-80 59 4 4 1.000 16.61
				,,,,,	55.551	4.000 10.01

- 66 -ANISOU 1617 CG2 THR 234 1564 1672 3077 3 -34 - 42 235 20.712 1618 N GLY9.441 37.833 1.000 15.80 ANISOU 1618 N GLY 235 1905 1914 2564 193 29 - 219 1619 CA GLY235 21.484 8.209 37.792 1.000 17.10 ANISOU 1619 CA GLY235 2049 1861 2586 133 223 - 4881620 C MOTA GLY 7.931 235 22.225 39.083 1.000 18.06 ANISOU 1620 C GLY 235 2046 2049 2768 419 499 3 0 3 1621 0 MOTA GLY 235 23.285 7.289 39.010 1.000 21.26 ANISOU 1621 O GLY 235 2167 2606 3303 679 343. - 74MOTA 1622 N GLY 236 21.602 8.149 40.237 1.000 15.17 ANISOU 1622 N GLY 236 1663 1901 2582 36 291 3 0 5 1623 CA GLY ATOM 236 22.080 7.673 41.520 1.000 17.27 ANISOU 1623 CA GLY 236 2135 1671 2754 225 1624 C 236 23.033 8.639 42.194 1.000 16.88 ATOM GLY 236 23.633 1.890 236 23.692 8.272 236 2165 2399 237 23.134 9.890 ANISOU 1624 C GLY 1890 2644 204 100 222 1625 O MOTA GLY 43.193 1.000 19.42 2814 314 -90 4 1 9 41.746 1.000 16.99 ANISOU 1625 O GLY MOTA 1626 N GLN 237 1647 ANISOU 1626 N GLN1851 2957 213 -213 1 6 7 10.849 42.298 1.000 16.75 ATOM 1627 CA GLN 237 24.074 ANISOU 1627 CA GLN 237 1608 2004 2752 72 177 9 8 237 23.481 ATOM 1628 C GLN 11.604 43.483 1.000 15.64 ANISOU 1628 C 237 1404 GLN 2136 2402 231 -146 2 0 0 1629 0 237 24.183 GLN 12:382 44.164 1.000 18.17 ANISOU 1629 O GLN 237 1581 2508 2817 -227 -6 - 4 6 MOTA 1630 CB GLN237 24.456 11.855 41.217 1.000 17.17 ANISOU 1630 CB GLN237 1912 2080 2532 71 141 - 7 237 25.304 1631 CG MOTA GLN11.221 40.115 1.000 17.64 ANISOU 1631 CG GLN 237 1850 2410 2441 226 95 - 30 1632 CD MOTA GLN237 25.721 12.302 39.137 1.000 19.72 ANISOU 1632 CD GLN237 1680 2833 2979 104 317 307 MOTA 1633 OE1 GLN 237 26.602 13.110 39.436 1.000 24.27 ANISOU 1633 OE1 GLN 237 1841 3145 4234 -213 -187 8 0 9 1634 NE2 GLN 237 24.986 12.399 38.027 1.000 18.53 ANISOU 1634 NE2 GLN 237 2007 2298 2735 432 374 202 ATOM 1635 N VAL 238 22.221 11.359 43.807 1.000 14.75 ANISOU 1635 N VAL 238 1563 -32 -54 4 1804 2237 MOTA 1636 CA VAL 238 21.533 12.075 44.862 1.000 14.41 ANISOU 1636 CA 238 1535 238 20.861 0 -44 3 2 VAL 1553 2388 1637 C MOTA VAL 11.060 45.781 1.000 13.56 ANISOU 1637 C VAL 238 1414 1392 2346 82 55 - 149 238 20.136 ATOM 1638 O VAL 10.174 45.302 1.000 15.87 238 1655 ANISOU 1638 O VAL 1639 2737 -218 -285 - 22238 20.467 MOTA 1639 CB 13.061 44.309 1.000 14.73 VAL ANISOU 1639 CB VAL 238 1817 35 - 437 - 95 1626 2152 1640 CG1 VAL 238 19.805 13.764 45.489 1.000 15.70 ANISOU 1640 CG1 VAL 238 1965 1490 2510 -524 - 423 174 1641 CG2 VAL 238 21.064 13.994 43.280 1.000 16.82 ANISOU 1641 CG2 VAL 238 1862 1718 2812 -60 -378 2 2 2 ATOM 1642 N LYS 239 21.119 11.153 47.071 1.000 14.47 ANISOU 1642 N LYS 239 1704 1474 2318 14 -40 1 2 1643 CA ATOM LYS 239 20.470 10.360 48.104 1.000 14.43 ANISOU 1643 CA LYS -168 1 7 9 239 1460 1617 2406 106 ATOM 1644 C LYS 239 19.048 10.852 48.409 1.000 14.82 ANISOU 1644 C LYS 239 1533 1456 -53 232 2642 102 1645 0 ATOM LYS 239 18.839 12.067 48.457 1.000 14.74 ANISOU 1645 O LYS 239 1841 1442 2318 158 LYS MOTA 1646 CB 239 21.320 10.435 49.385 1.000 16.40 ANISOU 1646 CB LYS 239 1995 -543 2 5 2 1712 2527 243 MOTA 1647 CG LYS 239 20.767 9.549 50.498 1.000 16.65 ANISOU 1647 CG 239 1954 LYS 1759 2614 -58 -781 2 4 4

									1 C1/GD/0/03000
						- 67 -			
ATOM	1648		LYS		21.738	9.511		1.000	19.76
ANISOU ATOM	1648 1649		LYS		2954	1820	2732	-123	-1234 363
ANISOU	1649		LYS LYS		21.107	8.835			22.58
ATOM	1650		LYS		3331	2164	3086	-652	
ANISOU			LYS		21.904 2817	8.883	54.145		23.13
ATOM	1651		ALA	240	18.140	3360 9.892	2612	-471	-943 2 8 7
ANISOU			ALA		1429	1607	2418	-156	14.35
ATOM	1652		ALA	240	16.791	10.192	49.145		-334 - 61 13.98
ANISOU	1652	CA	ALA		1468	1635	2210	-151	
ATOM	1653		ALA		16.728	9.776		1.000	13.44
ANISOU			ALA		1439	1388	2279	77 -4	50 2 2
ATOM	1654		ALA		16.514	8.592	50.913	1.000	16.32
ANISOU			ALA		1932	1567	2699	-215	-673 3 1 4
ATOM ANISOU	1655		ALA		15.712	9.565	48.268		15.21
ATOM	1656		ALA PRO	240	1510 16.907	1962	2306	-104	
ANISOU			PRO		1634	10.701 1551	51.546		14.23
ATOM	1657		PRO		17.035	10.251	2221	-87	-292 7 1
ANISOU			PRO		1718	1681	2180	-350	14.68 -174 - 30
MOTA	1658		PRO		15.693	9.961	53.579		13.89
ANISOU			PRO	241	1659	1581	2039	-107	
ATOM	1659		PRO		14.629	10.527		1.000	17.06
ANISOU			PRO		1698	1946	2838	17 - 2	54 146
ATOM ANISOU	1660 1660		PRO		17.689	11.462	53.619	1.000	16.63
ATOM	1661		PRO PRO		2162 17.138	1657	2501	-460	-487 5 5
	1661		PRO		-2433	12.651 1601	52.826 2258		16.56
ATOM	1662		PRO		17.164	12.140		-367 1 000	-274 3 1 14.92
ANISOU	1662	CD	PRO		1841	1490	2339	-215	-186 - 66
ATOM	1663		ARG		15.740	9.049			15.74
	1663		ARG		1914	1853	2212	-381	-308 2 0 4
ATOM ANISOU	1664		ARG		14.574	8.772	55.376		15.50
ANISOU	1664 1665		ARG		1955	1863	2073	-236	-291 1 8 0
	1665		ARG ARG		14.406 1889	9.841			16.60
ATOM	1666		ARG		15.372	2011 10.416	2407	-120	-411 - 5 1 18.31
ANISOU	1666		ARG		2041	2186	2732	-216	-559 - 180
ATOM	1667	CB	ARG		14.728	7.419			18.38
	1667		ARG	242	2920	1810	2253	-486	-391 2 6 9
MOTA	1668		ARG	242	14.564	6.273		1.000	18.42
ANISOU			ARG		2372	1873	2755	-88	162 - 155
ATOM ANISOU	1669 1669		ARG		14.854	4.935	55.796		23.07
ATOM	1670		ARG		3380	2022	3366	470	-483 -217
	1670		ARG ARG	242	16.334 3498	4.954			26.69
ATOM	1671		ARG		16.941	2727 3.921	3916	444	-829 4 7
	1671	CZ	ARG	242	3166	2879	56.584 4284	-297	-1143 802
ATOM	1672	NH1	ARG		16.157	2.913		1 000	33.14
ANISOU	1672	NH1	ARG		3810	3235	5546	-316	528 726
ATOM	1673	NH2	ARG		18.241	3.889			31.13
ANISOU	1673				3043	2925	5859	227	-769 4 8 4
ATOM ANISOU	1674		HIS	243	13.188	10.057			17.55
ATOM	1674 1675		HIS	243	1979	2233	2457	-165	-173 - 74
	1675		HIS		12.913	11.050	57.914		17.84
ATOM	1676		HIS HIS	243	2186 11.644	2139	2452	-260	-123 - 75
	1676		HIS		2102	10.627 2084			17.52
ATOM	1677		HIS		10.870	9.803	2470 58.132	-248	-164 - 325 20.23
	1677	0	HIS		2226	2593	2868	-551	-323 - 392
ATOM	1678	СВ	HIS		12.865	12.456			19.74

- 68 -ANISOU 1678 CB HIS 243 2770 2248 2482 -188 -106 8 3 1679 CG HIS 243 11.922 12.630 56.187 1.000 22.60 HIS ANISOU 1679 CG 243 3449 2513 2624 164 -382 0 1680 ND1 HIS ATOM 243 12.209 12.299 54.879 1.000 25.87 ANISOU 1680 ND1 HIS 243 4780 2575 -609 2473 -403 5 3 MOTA 1681 CD2 HIS 243 10.633 13.034 56.172 1.000 29.11 ANISOU 1681 CD2 HIS 243 3220 4490 3348 121 -421 1630 1682 CE1 HIS ATOM 243 11.182 12.573 54.109 1.000 32.92 ANISOU 1682 CE1 HIS 243 5835 3672 3001 -1102 -1367 689 243 10.214 13.012 1683 NE2 HIS 54.875 1.000 36.95 ANISOU 1683 NE2 HIS 243 5719 4201 4119 1019 -2016 987 1684 N HIS 244 11.437 11.194 59.831 1.000 18.87 ANISOU 1684 N HIS 244 2523 2477 2171 -88 -141 - 1171685 CA HIS 244 10.302 10.801 60.649 1.000 20.83 244 2802 2485 244 9.927 11.968 244 1803 2969 ANISOU 1685 CA HIS 2628 171 251 272 1686 C HIS 11.968 61.551 1.000 20.33 ANISOU 1686 C HIS 2953 -31 -78 1687 O HIS ATOM 244 10.482 13.073 61.510 1.000 21.71 244 2057 3418 2774 -535 145 -244 10.714 9.557 61.468 1.000 24.38 244 4066 2644 2553 -76 -390 4 ANISOU 1687 O HIS 145 -853 1688 CB HIS ANISOU 1688 CB HIS -390 4 4 1 1689 CG HIS 244 11.859 9.725 62.423 1.000 28.34 244 4158 3498 3113 696 -727 -ANISOU 1689 CG HIS -727 - 8 9 244 13.132 9.205 62.268 1.000 32.35 244 4012 4471 3808 548 -485 -1690 ND1 HIS ANISOU 1690 ND1 HIS -485 - 850 MOTA 1691 CD2 HIS 244 11.928 10.391 63.609 1.000 25.21 244 2937 4137 2505 -373 45 21 9 244 13.887 9.531 63.312 1.000 31.71 244 4157 4277 3613 1224 -749 -518 244 13.146 10.263 64.150 1.000 24.52 ANISOU 1691 CD2 HIS ATOM 1692 CE1 HIS ANISOU 1692 CE1 HIS HIS 244 13.146 10.263 64.150 1.000 24.52
HIS 244 3165 3517 2633 94 -82 4 9 2
VAL 245 8.890 11.687 62.349 1.000 23.87
VAL 245 2627 3119 3322 -251 531 -310
VAL 245 8.473 12.691 63.349 1.000 24.85
VAL 245 2785 3770 2888 481 149 -293
VAL 245 8.624 12.079 64.735 1.000 26.03
VAL 245 3220 3558 3112 -289 179 8 9
VAL 245 8.023 11.025 64.969 1.000 27.98
VAL 245 3120 3085 4428 42 295 -59
VAL 245 7.020 13.114 63.099 1.000 26.02
VAL 245 2621 3489 3777 94 -103 -569
VAL 245 6.586 14.114 64.161 1.000 28.06
VAL 245 3564 3809 4220 1264 -305 - 33
ALA 246 9.399 12.696 65.603 1.000 28.08
ALA 246 4338 3787 2543 -850 250 254 MOTA 1693 NE2 HIS ANISOU 1693 NE2 HIS ATOM 1694 N ANISOU 1694 N VAL 1695 CA VAL ANISOU 1695 CA VAL 1696 C ANISOU 1696 C ATOM 1697 O ANISOU 1697 O 1698 CB MOTA VAL ANISOU 1698 CB VAL ATOM 1699 CG1 VAL ANISOU 1699 CG1 VAL ATOM 1700 CG2 VAL ANISOU 1700 CG2 VAL ATOM 1701 N ANISOU 1701 N ALA 246 4338 3787 2543 -850 250 2 ALA 246 9.567 12.316 67.003 1.000 27.45 -850 250 254 1702 CA ALA MOTA ANISOU 1702 CA ALA 246 4363 3360 2707 275 373 292 1703 C ALA246 8.356 12.740 67.833 1.000 32.68 ANISOU 1703 C 246 4915 4473 ALA3031 98 880 1 9 7 ATOM 1704 O 246 7.774 13.791 67.563 1.000 29.54 ALA ANISOU 1704 O ALA246 3522 4283 3417 -224 875 -329 1705 CB ALA ATOM 246 10.819 13.010 67.542 1.000 30.33 ANISOU 1705 CB ALA
 246
 4564
 3949
 3011
 615
 -221

 247
 8.048
 11.958
 68.849
 1.000
 34.09
 3011 615 -221 - 422 ATOM 1706 N ALA 247 4483 5156 247 7.036 12.190 ANISOU 1706 N ALA 3311 -1190 466 3 9 3 ATOM1707 CA ALA 12.190 69.859 1.000 34.23 ANISOU 1707 CA ALA247 4188 5627 3189 -1215 315 515

4684

247 5419

247 7.609 12.910 71.081 1.000 33.31

2555

249

-506 1147

1708 C

ANISOU 1708 C

ALA

ALA

ATOM

				- 69 -			
ATOM ANISOU ATOM	1710 CB 1711 N 1711 N 1711 N 1712 CA 1713 C 1713 C 1714 O 1715 CB 1716 CG 1717 CD 1717 CD 1718 N 1719 CA 1719 CA 1720 C 1721 O 1722 CB 1722 CG 1721 CD 1722 CB 1723 CC 1721 CD 1722 CB 1723 CC 1721 CD 1722 CB 1723 CC 1724 CD 1725 NE 1726 CZ 1727 NH	ALAAAOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO	247 8.787 247 6.388 247 6.388 247 6.388 248 6.817 248 577.256 248 75.68 248 75.68 248 7651 248 6.251 248 8563 248 8563 248 8563 248 8563 248 8563 248 8563 248 8563 248 8563 248 8563 248 6395 249 9141 249 9141 249 75.249 249 77.249 249 86.244 249 99.881 249 10.269 249 12.297	12.4 10.2 10.2 10.2 10.3	4259 70.314 2801 71.577 4836 72.73 3996 73.948 5075 74.014 4237 72.89 75523 72.29 6545 76.114 606 74.883 76.916 3568 77.831 7433 76.721 4326 76.110 6779 77.165 7984 76.580 8271 77.282 78.521	-378 1.000 -2800 1.000 -300 1.000 -645 1.000 -1446 1.000 -1127 1.000 -513 1.000 -1317 1.000 -1317 1.000 -1317 1.000 -1317 1.000 -1317 1.000 -2484 1.000 -377 1.000 -377 1.000 2171 1.000 2362 1.000 2304	552 985 45.48 2573 - 796 49.75 1238 - 138 50.89 2210 - 1064 44.69 953 - 577 48.76 1069 - 477 55.51 895 566 46.09 -7 1237 56.25 1799 3995 55.24 2864 1270 71.04 3707 622 72.89 2723 409 70.73 2650 - 266 72.71 2153 133
ATOM	1718 N 1718 N	ARG	249 8.109	13.683	6006 74.883	937 1.000	953 - 577 48.76
ANISOU	1719 CA	ARG ARG	249 7.865 249 10023	12.783 6914	76.024 4156	1.000 -1098	55.51 895 566
ANISOU ATOM	1720 C 1721 O	ARG ARG	249 5561 249 6.244	8382 12.915	3568 77.831	-2484	-7 1237
ATOM ANISOU	1722 CB 1722 CB	ARG ARG	249 9.177 249 8950	12.459	76.721	1.000	55.24
ANISOU ATOM	1723 CG 1724 CD	ARG	249 12881	7330	76.110 6779	1.000 1135	71.04 3707 622
ATOM	1725 NE 1725 NE	ARG	249 11.124	7991 9.162	7984 76.580	2171 1.000	2723 4 0 9 70.73
ANISOU ATOM	1726 CZ 1727 NH1	ARG ARG	249 12.039 249 10269	8.493 9417	77.282 7942	1.000 2304	72.71 2153 1 3 3
\mathtt{ATOM}	1727 NH1 1728 NH2 1728 NH2	ARG	249 22286 249 12.682 249 5358	6161 7.462 10062	5559 76.761 10295	2015	1622 3 8 7 4 6 7 . 6 8
ATOM ANISOU ATOM	1729 N	ALA ALA ALA	254 1.981 254 15501 254 2.287	18.918 7922	75.430 8964	-4581	3886 2 2 1 8 5 . 2 4 -1437 2 3 4 7
	1730 CA 1731 C 1731 C	ALA ALA ALA	254 12510 254 2.943	20.081 8110 21.216	76.257 8286 75.489	-3993 1.000	1617 1592 60.91
ATOM	1732 O 1732 O 1733 CB	ALA ALA	254 8383 254 4.174 254 8056	5719 21.309 8109	9040 75.487 11332	1602	4553 3381
	1733 CB 1734 N	ALA ALA GLY	254 3.264 254 12589 255 2.200	19.667 7262 22.108	77.351 3131 74.846	-866 1.000	4570 - 1112 54.40
ATOM ANISOU ATOM	1735 CA 1735 CA	GLY GLY	255 8029 255 2.880 255 5181	5451 23.171 4570	7190 74.098 5465	1424	2922 - 940 40.05 836 - 921
	1736 C 1736 C 1737 O	GLY GLY	255 3.640 255 4227 255 4.580	22.565 4772 23.163	72.921 5749 72.398	557 1.000	38.82 702 -1561 39.96
ATOM ANISOU		GLY SER SER	255 2978 256 3.164 256 5047	6491 21.387 4594	5715 72.509 4527	-128	-136 -2226
MOTA	1739 CA	SER	256 3.738	20.606	71.429		35.71

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						70			
ANISOU			SER	256	4737	4533	4299	560	-501 - 919
ATOM	1740	С	SER		2.983	20.742	70.118		
ANISOU			SER		4584	4669			34.93
ATOM	1741						4019	-98	-85 9 1
		_	SER	256	3.251	20.000	69.162	1.000	33.92
ANISOU			SER	256	3575	6107	3207	503	304 377
\mathtt{ATOM}	1742	CB	SER	256	3.845	19.136	71.853		
ANISOU	1742	CB	SER	256	3125	4830	3509		
ATOM	1743		SER	256				624	212 - 492
ANISOU					2.688	18.752	72.601		61.15
			SER	256	2987	8497	11750	451	1943 2630
ATOM	1744		SER	257	2.065	21.700	70.030	1.000	35.54
ANISOU	1744	N	SER	257	4037	5989	3479	347	242 - 86
ATOM	1745	CA	SER	257	1.379	21.993	68.767		242 - 6 6
ANISOU	1745	CA	SER	257	2824	5827	3100		
ATOM	1746		SER	257			3109	170	672 - 509
ANISOU					2.378	22.538	67.760	1.000	30.63
			SER	257	3181	5524	2934	-476	765 -1297
MOTA	1747		SER	257	3.359	23.159	68.199	1,000	34.70
ANISOU			SER	257	3500	6070	3616	-829	603 -1516
ATOM	1748	CB	SER	257	0.331	23.088	69.036		38.70
ANISOU	1748	CB	SER		3085	6518			
ATOM	1749		SER		0.801		5103	796	1381 4 3 5
ANISOU				257	0.801	24.361	68.601		
			SER	25/	8002	5175	11565	-999	-3375 383
ATOM	1750		ARG	258	2.119	22.384	66.471	1.000	30.51
ANISOU			ARG	258	3668	5068	2855	-332	677 - 995
ATOM	1751		ARG	258	2.997	22.819	65.396		28 15
ANISOU	1751	CA	ARG		3100	4620	2976	-106	358 - 544
ATOM	1752		ARG		2.198	22.913			
	1752		ARG		3488		64.096		
ATOM	1753			250	3400	3381	2872	-676	273 - 904
			ARG	258	1.132	22.294	63.981		
	1753	0	ARG		3162	3240	3070	-441	478 - 560
ATOM	1754		ARG		4.175	21.873	65.154	1,000	27.21
ANISOU	1754	CB	ARG	258	3158	4041	3141	-446	313 -1352
ATOM	1755	CG	ARG		3.861	20.508	64.570		30 00
ANISOU	1755		ARG		4782	3429			
ATOM	1756		ARG		5.039		3531	-737	-738 - 389
	1756	CD				19.537	64.769		
ATOM	1720	CD	ARG		5937	3466	4523	106	477 306
	1757		ARG	258	4.597	18.176	64.411	1.000	32.42
	1757		ARG		3372	3858	5089	-85	-274 5 2 8
\mathtt{ATOM}	1758		ARG	258	4.633	17.777	63.143		
LOSIKA	1758	CZ	ARG		5670	2958	5553	155	680 4 3
ATOM	1759	NH1	ARG	258	5.075	18.622	62.217		
ANISOU	1759	NH1	ARG	250	3077		4001		
ATOM	1760	רעות	A D.C			3435	4881	-150	-211 -103
	1760	NILLO	DAM		4.210	16.566	62.824		38.66
ANISOU	1700	NHZ	ARG		5812	3151	5724		-1632 865
ATOM	1761		THR	259	2.806	23.572	63.120	1.000	23.62
ANISOU			THR	259	2625	3578	2771	-519	315 -1037
MOTA	1762	CA	THR		2.337	23.482	61.730		
ANISOU	1762	CA	THR	259	2614	2934			
ATOM	1763		THR	250	3.528		2800	-36	247 -1041
ANISOU			THR	255		23.197	60.808		
ATOM	1764			259		2663	2587	-38	21 -699
			THR	259	4.698	23.411	61.159	1.000	21.13
	1764		\mathtt{THR}	259	2464	3096	2468	-495	
ATOM	1765	СB	THR	259	1.682	24.793	61.278		
ANISOU	1765	CB	THR	259	2125	3084	3927		57 -1229
ATOM	1766	OG1	THR	259	2.697	25.790			
ANISOU	1766	OG 1	THR	250	2297		61.041		
ATOM	1767	CGS	מעת	250	0 700	2848	3648	196	-142 - 829
ANISOU	1767	CC2	መጠጋ ተተተፈ	433	0.760	25.408			25.17
ATOM				259		3229	3393	726	264 - 136
	1768		SER	260	3.234	22.706		1.000	20.41
	1768		SER		2386	2762	2609	-61	74 -806
MOTA	1769		SER	260	4.225	22.515			19.33
ANISOU	1769	CA	SER		2488	2459	2399	192	8 - 344
				-			200		U - J + 4

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1770 C
MOTA
                SER
                     260 3.587
                                 22.871
                                        57.210 1.000 18.78
ANISOU 1770 C
                SER
                     260 1996
                                 2544
                                         2595
                                                -379 -264 - 311
       1771 0
                SER
                     260 2.375
                                 22.758
                                         56.988 1.000 21.20
ANISOU 1771 O
                SER
                     260 1917
                                 2448
                                         3689
                                                -75
                                                      -269 - 573
ATOM
       1772 CB
                     260 4.738
                SER
                                 21.076
                                        58.480 1.000 20.28
ANISOU 1772 CB
                SER
                     260 2491
                                 2458
                                         2755
                                                160
                                                      -101 - 495
       1773 OG
MOTA
                SER
                     260 3.656
                                         58.227 1.000 22.70
                                 20.197
ANISOU 1773 OG
                SER
                     260 2758
                                 2574
                                         3294
                                                -113 -234 - 169
ATOM
       1774 N
                                 23.329 56.330 1.000 18.79
                SER
                     261 4.474
ANISOU 1774 N
                SER
                     261 2189
                                 2215
                                         2737
                                                -55
                                                     -92 3 5
       1775 CA
MOTA
                SER
                     261 4.148
                                 23.585
                                        54.929 1.000 16.88
ANISOU 1775 CA
               SER
                     261 2074
                                 1718
                                         2622
                                                22 -117 -404
       1776 C
ATOM
                SER
                     261 5.066
                                 22.672
                                        54.106 1.000 17.25
ANISOU 1776 C
                SER
                     261 1720
                                 1833
                                         3000
                                                101
                                                      -350 - 491
       1777 O
MOTA
                SER
                     261 6.272
                                 22.876 54.173 1.000 19.96
ANISOU 1777 O
                SER
                     261 1712
                                2417
                                         3456 . 50 -483 -781
       1778 CB
ATOM
                SER
                     261 4.471 25.028 54.503 1.000 19.95
ANISOU 1778 CB
                SER
                     261 2903
                                1675
                                         3002
                                                164
                                                      -113 - 135
       1779 OG
                SER
                     261 4.404 25.127
                                        53.107 1.000 35.64
ANISOU 1779 OG
                    261 5435
               SER
                                4814
                                         3293
                                                -1089 -766 1263
MOTA
       1780 N
                VAL
                    262 4.467
                                 21.722 53.435 1.000 15.56
ANISOU 1780 N
                VAL
                     262 1751
                                 2021
                                         2140
                                                -75
                                                      -40 - 436
       1781 CA
ATOM
               VAL
                     262 5.247
                                 20.713
                                        52.711 1.000 15.41
ANISOU 1781 CA
               VAL
                     262 1871
                                1938
                                         2048
                                                43 21 - 196
MOTA
       1782 C
                VAL
                     262 4.914
                               20.874
                                        51.242 1.000 14.05
ANISOU 1782 C
                VAL
                     262 1460
                                 1784
                                         2095
                                                -13
                                                      29 - 144
                     262 3.759
262 1488
262 4.902
       1783 O
ATOM
                VAL
                                 20.712
                                        50.844 1.000 15.45
ANISOU 1783 O
                VAL
                                 1900
                                         2481
                                                -175 -94 -191
       1784 CB
               VAL
                                 19.307
                                        53.253 1.000 16.87
ANISOU 1784 CB VAL
                     262 2144
                                 2005
                                         2260
                                                165
                                                     -164 2 3
       1785 CG1 VAL
                     262 5.567
                                 18.275
                                        52.364 1.000 20.01
ANISOU 1785 CG1 VAL
                     262 2433
                                 2006
                                         3165
                                                4 -191 -637
       1786 CG2 VAL
                     262 5.335
                                 19.200
                                         54.715 1.000 18.63
ANISOU 1786 CG2 VAL
                     262 2390
                                                     -397 1 7 5
                                 2242
                                         2446
                                                147
ATOM
       1787 N
               PHE
                     263 5.894
                                 21.163
                                         50.412 1.000 13.73
ANISOU 1787 N
                PHE
                     263 1497
                                 1573.
                                         2148
                                                5 -64 1 8 6
ATOM
       1788 CA PHE
                     263 5.762
                                 21.411
                                         48.994 1.000 13.04
ANISOU 1788 CA
               PHE
                     263 1654
                                 1196
                                         2105
                                                -12
                                                      -193 1 1 3
MOTA
       1789 C
                PHE
                     263 6.479
                                 20.253
                                         48.284 1.000 13.56
ANISOU 1789 C
               PHE
                     263 1432
                                 1351
                                         2370
                                                -175
                                                      -98
MOTA
       1790 O
               PHE
                     263 7.732
                                 20.177
                                         48.281 1.000 13.83
ANISOU 1790 O
               PHE
                     263 1415
                                 1437
                                         2403
                                                -82
                                                      -299 - 104
ATOM
       1791 CB
               PHE
                     263 6.364
                                 22.770
                                        48.594 1.000 13.50
ANISOU 1791 CB
               PHE
                     263 1658
                                1374
                                         2098
                                                -295
                                                      -97
MOTA
       1792 CG
               PHE
                     263 6.062
                                 23.148
                                        47.135 1.000 13.34
ANISOU 1792 CG PHE
                     263 1616
                                1358
                                         2096
                                                -159
                                                      -111 8 2
       1793 CD1 PHE
ATOM
                     263 6.750
                               22.635
                                        46.051 1.000 14.95
ANISOU 1793 CD1 PHE
                     263 1977
                                1547
                                         2156
                                                -354
                                                     -131 - 384
ATOM
       1794 CD2 PHE
                     263 5.005
                                24.048
                                        46.883 1.000 15.37
ANISOU 1794 CD2 PHE
                     263 1549
                                1557
                                         2735
                                                -139
                                                      -264 3 0 3
       1795 CE1 PHE
MOTA
                     263 6.468
                                 22.945
                                         44.720 1.000 14.58
ANISOU 1795 CE1 PHE
                     263 1721
                                1621
                                         2196
                                                -242 71 - 144
MOTA
       1796 CE2 PHE
                     263 4.703
                                 24.366
                                         45.566 1.000 14.71
ANISOU 1796 CE2 PHE
                     263 1482
                                 1428
                                         2680
                                                -20
                                                      -261 1 3 7
ATOM
       1797 CZ
                PHE
                     263 5.383
                                 23.809
                                         44.479 1.000 16.55
ANISOU 1797 CZ
                PHE
                     263 1935
                                 1492
                                         2862
                                                -152
       1798 N
ATOM
                PHE
                     264 5.721
                                 19.405
                                         47.588 1.000 12.07
ANISOU 1798 N
                PHE
                     264 1277
                                 1343
                                         1967
                                                -66
MOTA
       1799 CA
                PHE
                     264 6.267
                                 18.328 46.769 1.000 11.90
ANISOU 1799 CA
                PHE
                     264 1177
                                 1289
                                         2058
                                                -129
                                                      34 - 21
       1800 C
                PHE
                     264 6.440
                               18.775 45.314 1.000 11.76
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						- 72 -		
ANISOU			PHE		1206	1258	2004	-121 -42 8
ATOM	1801		PHE		5.418	19.097		1.000 12.55
ANISOU			PHE		1165	1473	2133	-77 -120 4 6
ATOM	1802		PHE	264	5.346	17.099		1.000 12.39
ANISOU			PHE	264	1101	1498	2110	-304 -42 6 3
ATOM	1803	CG	PHE	264	5.022	16.558		1.000 13.97
ANISOU			PHE		1647	1465	2197	-290 13 1 2 1
ATOM	1804	CD1	PHE		5.960	15.848		1.000 17.07
ANISOU		CD1	PHE	264	2039	1976	2471	-422 -410 4 9 7
MOTA	1805	CD2	PHE	264	3.747	16.679		1.000 17.41
ANISOU		CD2	PHE	264	1835	2359		
ATOM			PHE	264	5.661	15.247	50 053	-440 433 112 1.000 20.59
ANISOU		CEl	PHE	264	2616	2710	2496	-556 -425 7 2 5
MOTA	1807	CE2	PHE	264	3.458	16.133		1.000 22.51
ANISOU				264	2151	4047	2355	-787 106 553
ATOM	1808		PHE	264	4.386	15.350		1.000 20.88
ANISOU			PHE	264	2889	2376	2669	-936 - 22 3 0 6
ATOM	1809		LEU	265	7.676	18.756		1.000 11.81
ANISOU			LEU	265		1248	2047	-37 47 1 9
ATOM	1810	CA	LEU	265	7.900	19.000		1.000 12.01
ANISOU	1810	CA	LEU	265	1264	1269	2028	-223 16 - 63
ATOM	1811	С	LEU	265	7.915	17.617		1.000 12.10
ANISOU			LEU	265	1266	1298	2033	-117 -81 3
ATOM	1812		LEU	265	8.842	16.834		1.000 12.93
ANISOU			LEU	265	1367	1283		-107 -152 4 4
ATOM	1813		LEU		9.246	19.730	43.156	1.000 12.59
ANISOU ATOM			LEU	265		1364	2019	-257 57 - 9
ANISOU	1814	CG	LEU	265	9.500	20.124	41.709	1.000 12.19
ATOM			LEU	265	1168	1399	2066	-292 -248 3 0 2
ANISOU	1815	CDI	LEU		8.620	21.314	41.318	1.000 13.29
ATOM	1816	CDI	PEO	265	1518	1546	1984	84 36 1 9
ANISOU	1016	CDZ	LEU	265	10.971	20.458	41.449	1.000 13.14
ATOM	1817				1204	1593	2197	-234 41 - 20
ANISOU			ARG ARG		6.842	17.249	41.996	1.000 12.06
ATOM	1818		ARG	266	1412	1127	2043	-220 -190 4 5
ANISOU	1818	CV	ARG	200	6.586	15.913	41.488	1.000 12.07
ATOM	1819		ARG		1372 6.619	1201	2012	-258 0 8 0
ANISOU			ARG	200	1203	15.965	39.972	1.000 11.75
ATOM	1820		ARG		6.032	1315	1948	29 -267 142
ANISOU	1820	Ô	ARG		1430	16.860	39.396	1.000 13.06
ATOM	1821	СB	ARG	266	5.243	1318 15.370	2214	5 -173 281
ANISOU	1821	CB	ARG	266	1142	1477	41.994	1.000 12.95
ATOM	1822	CG	ARG		5.036	15.606	2302	-189 43 - 33
ANISOU	1822	CG	ARG		1351	1686	43.488 2207	1.000 13.80
ATOM	1823	CD	ARG		3.723	15.041		-159 66 -115
ANISOU	1823	CD	ARG	266	1369	1362	2094	1.000 12.70 66 -22 8 4
MOTA	1824	NE	ARG		2.581	15.648	43.281	1.000 12.97
ANISOU	1824	ΝE	ARG	266	1343	1155	2428	52 -165 -137
MOTA	1825	CZ	ARG		1.304	15.281		1.000 11.34
ANISOU			ARG		1432	1009	1869	45 -149 -103
ATOM	1826	NH1	ARG		0.995	14.414		1.000 13.39
ANISOU	1826	NH1	ARG	266	1802	1165	2119	-11 -38 7 2
ATOM	1827	NH2	ARG		0.305	15.821		1.000 12.55
ANISOU	1827	NH2	ARG	266	1490	1067	2210	125 -357 - 159
\mathtt{ATOM}	1828	N	PRO	267	7.237	14.951	39.357	1.000 12.74
ANISOU			PRO	267	1418	1394	2030	16 -146 108
ATOM	1829	CA	PRO	267	7.298	14.947	37.887	1.000 13.88
	1829		PRO	267	1442	1786	2047	167 -125 - 84
ATOM	1830	С	PRO	267	5.957	14.722	37.222	1.000 12.61
ANISOU	1830	С	PRO	267	1413	1508	1868	-6 44 2 7
							-	'

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- 74 -
 ANISOU 1861 CG PHE 271 1729
                                     1320
                                              2485
                                                      -152 34 -124
                      271 11.460 12.369
         1862 CD1 PHE
                                              33.814 1.000 17.76
 ANISOU 1862 CD1 PHE
                        271 1714
                        271 1714 1581
271 10.698 10.972
                                              3452
                                                      -235 393 -249
         1863 CD2 PHE
                                              35.570 1.000 18.04
 ANISOU 1863 CD2 PHE
                        271 2182
                                     1543
                                              3130
                                                      -95
         1864 CE1 PHE
                                                             -540 1 7 2
                        271 12.786 12.092
                                              34.166 1.000 17.54
 ANISOU 1864 CE1 PHE
                        271 1838
                                     1700
                                              3128
                                                      -291
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 ATOM
         1865 CE2 PHE
                        271 11.997 10.609
                                              35.899 1.000 18.84
 ANISOU 1865 CE2 PHE
                        271 1935
                                     1646
                                              3578
                                                      -392
                                                            -396 4 2 5
 ATOM
         1866 CZ PHE
                        271 13.039 11.154
                                             35.162 1.000 17.25
ANISOU 1866 CZ PHE
                       271 2444
                                     1697
                                              2415
                                                      -485
                                                            -19 -394
 ATOM
         1867 N
                  THR
                       272 10.278 10.298
                                             31.453 1.000 13.78
 ANISOU 1867 N
                  THR
                       272 1514 1641
                                              2083
                                                     30 19 154
 ATOM
        1868 CA THR
                       272 10.811 9.046
272 1551 1660
                                              30.938 1.000 13.99
ANISOU 1868 CA THR
                                              2105
                                                     -99
                                                           83 6 7
        1869 C
                       272 12.246 8.841 31.410 1.000 14.71
                  THR
ANISOU 1869 C
                 THR
                       272 1598 1549
                                            2441
                                                     -3 108 3 5 7
 ATOM
        1870 O
                       272 13.046 9.808 31.424 1.000 16.23
                 THR
 ANISOU 1870 O
                       272 1646 1742 2780
                  THR
                                                     -246
        1871 CB THR
 ATOM
                       272 10.751 9.117 29.388 1.000 16.27
ANISOU 1871 CB THR
                      272 1856 2205 2119 191 125 8
272 9.341 9.221 29.032 1.000 17.99
272 1996 2473 2368 64 -190 264
272 11.249 7.856 28.723 1.000 17.94
ATOM
        1872 OG1 THR
ANISOU 1872 OG1 THR
ATOM
        1873 CG2 THR
ANISOU 1873 CG2 THR
                       272 2423
                      272 2423 2167 2227 173 177 - 273 12.567 7.600 31.743 1.000 14.91
                                                     173 177 - 94
ATOM
        1874 N
                 PHE
ANISOU 1874 N
                  PHE
                      273 1644
                                    1521 2499 92 238 2 1 8
7.253 32.254 1.000 15.16
        1875 CA PHE
                      273 13.894 7.253
MOTA
ANISOU 1875 CA PHE
                      273 1602 1813
                 PHE 273 1602 1813 2345 296 277 5
PHE 273 14.350 5.899 31.724 1.000 14.69
                                                     296 277 5 5
ATOM
        1876 C
ANISOU 1876 C
                 PHE 273 1408 1647
                      273 1408 1647 2528 24 479 1 78
273 13.541 5.086 31.262 1.000 15.91
273 1738 1767 2541 -115 450 1 1 9
273 1758 1921 2314 -344 286 1 2 3
273 12.931 6.336 34.424 1.000 14.54
273 13.601 6.743 2410 -95 -11 1 9 5
273 1457 2343 2521 2340 2360 2 6
ATOM
        1877 O
                 PHE
ANISOU 1877 O
                 PHE
ATOM
        1878 CB
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ANISOU 1878 CB
                 PHE
        1879 CG
                 PHE
ANISOU 1879 CG PHE
        1880 CD1 PHE
ANISOU 1880 CD1 PHE
                       273 1457 2343
                                            2521 -24
                                                            308 362
ATOM
        1881 CD2 PHE
                       273 13.295 5.038 34.721 1.000 15.23
ANISOU 1881 CD2 PHE
                       273 1863 1624
                                            2300
                                                     -110 91 136
        1882 CE1 PHE
                       273 10.719 5.848 35.259 1.000 16.10
ANISOU 1882 CE1 PHE
                       273 1593 2158
273 12.419 4.148
                                            2365 -162 292 122
        1883 CE2 PHE
                                           35.354 1.000 16.01
ANISOU 1883 CE2 PHE
                      273 1904 1980
273 11.109 4.559
                                           2198 -139 285 1
35.548 1.000 15.18
                                                    -139 285 181
ATOM
        1884 CZ
                 PHE
ANISOU 1884 CZ
                      273 1843
                 PHE
                                    2001
                                            1925
                                                     -141 73 - 227
ATOM
        1885 N
                      274 15.634 5.612
274 1559 1940
                 SER
ANISOU 1885 N
                                           31.926 1.000 15.31
                 SER
                                           2317 361 383 2
31.518 1.000 15.37
                                    1940
                                                           383 247
ATOM
        1886 CA
                      274 16.221 4.318
                 SER
ANISOU 1886 CA
ATOM 1887 C
                      274 1476 1723
274 15.953 3.284
                 SER
                                             2642 32 557 1 5 6
                 SER
                                             32.588 1.000 14.67
ANISOU 1887 C
                      274 973 1877 2726 -113 265 3 0 2
                 SER
ATOM
       1888 0
                      274 16.310 3.476 33.770 1.000 15.98
                 SER
ANISOU 1888 O
                 SER
                      274 1668
                                    1677
                                             2728
                                                     126
                                                           143 193
       1889 CB
                 SER
                      274 17.742 4.556
                                             31.356 1.000 17.41
ANISOU 1889 CB
                 SER
                      274 1487
                                    2019
                                             3112
                                                     235
                                                           945 725
       1890 OG
                      274 18.362 3.280
                 SER
                                             31.334 1.000 18.03
ANISOU 1890 OG
                 SER
                      274 1839
                                    1961
                                             3052
                                                     293
                                                           840 188
       1891 N
ATOM
                 VAL
                       275 15.395 2.133
                                             32.182 1.000 15.58
ANISOU 1891 N
                       275 1646
                 VAL
                                    1857
                                            2417
                                                     -182
                                                           461 261
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ATOM 1892 CA VAL 275 15.158 1.032 33.137 1.000 15.65 5 ANISOU 1892 CA VAL 275 1681 1800 2466 -180 261 2 6 5 ATOM 1893 C VAL 275 16.454 0.445 31.659 1.0001 15.35 3 ANISOU 1893 C VAL 275 16.623 0.280 31.659 1.0001 15.35 3 ANISOU 1894 O VAL 275 2037 1655 2267 6 297 196 ATOM 1895 CS VAL 275 16.623 0.280 31.001 15.65						1 C 17 G D 7 G 7 G 5 G G G
ANISOU 1892 CA VAL 275 1681 1800 2416 1893 C VAL 275 16.454 ANISOU 1893 C VAL 275 16.454 ANISOU 1893 C VAL 275 18.05 ANISOU 1894 O VAL 275 16.623 ANISOU 1894 O VAL 275 16.623 ANISOU 1895 CB VAL 275 16.623 ANISOU 1895 CB VAL 275 16.623 ANISOU 1895 CB VAL 275 16.35 ANISOU 1896 CG1 VAL 275 16.35 ANISOU 1896 CG1 VAL 275 16.35 ANISOU 1897 CG2 VAL 275 16.35 ANISOU 1897 CG2 VAL 275 16.50 ANISOU 1898 N PRO 276 19.27 100 ANISOU 1899 CA PRO 276 19.98 ANISOU 1900 C PRO 276 19.98 ANISOU 1900 C PRO 276 19.98 ANISOU 1901 C PRO 276 19.98 ANISOU 1901 CD PRO 276 19.98 ANISOU 1902 CB PRO 276 18.852 ANISOU 1903 CC PRO 276 18.852 ANISOU 1904 CD PRO 276 19.32 ANISOU 1905 CA LEU 277 19.325 ANISOU 1906 CA LEU 277 19.325 ANISOU 1907 CA LEU 277 19.325 ANISOU 1908 CA LEU 277 20.396 ANISOU 1909 CA LEU 277 20.396 ANISOU 1909 CA LEU 277 20.596 ANISOU 1901 CA ALA 278 17.86 ANISOU 1901 CA ALA 277 19.325 ANISOU 1902 CB PRO 276 18.852 ANISOU 1903 CA LEU 277 19.325 ANISOU 1903 CA LEU 277 19.325 ANISOU 1904 CA ALA 278 17.875 ANISOU 1905 CA LEU 277 20.396 ANISOU 1907 CA LEU 277 20.396 ANISOU 1908 CA LEU 277 20.396 ANISOU 1909 CA LEU 277 20.396 ANISOU 1901 CA ALA 278 17.575 ANISOU 1901 CA ALA 278 17.575 ANISOU 1901 CA ALA 278 17.575 ANISOU 1901 CA ALA 278 17.576 ANISOU 1901 CA ALA 278 17.576 ANISOU 1901 CA ARG 279 19.477 ANISOU 1901 CA ARG 279 19.477 ANISOU 1902 CA ARG 279 19.9477 ANISOU 1902 CA ARG 279 19.9477 ANISOU 1901 CA ARG 279 19.9477 ANISOU 1902 CA ARG 279 19.9477 ANISOU 1902 CA ARG 279 19.9477 ANISOU 1901 CA ARG 279 19.9477 ANISOU 1902 CA ARG 279 19.9477 ANISOU 1901 CA ARG 279 19.9477 ANISOU 1902 CA ARG 279 19.9477 ANISOU 1902 CA ARG 279 19.9477 A						
ANTON 1893 C VAL 275 1631 1800 2466 -180 261 2 65 ATOM 1893 C VAL 275 16.454 0.445 33.6599 1.0000 15.33 ANISOU 1893 C VAL 275 16.454 0.445 33.6599 1.000 15.33 ANISOU 1894 O VAL 275 16.623 0.280 34.871 1.000 15.68 26 26 26 26 27 27 29 20 27 20 28 26 27 6 29 7 1 9 6 27 27 20 27 20 27 20 28 27 28 28 27 28 28 27 28 28 28 28 28 28 28 28 28 28 28 28 28				1.033	33.137	1.000 15.65
ANISOU 1893 C VAL 275 16.649 0.445 33.659 1.000 15.33 ANISOU 1894 0 VAL 275 16.623 0.280 34.871 1.000 15.68 ANISOU 1894 0 VAL 275 16.623 0.280 34.871 1.000 15.68 ANISOU 1895 CB VAL 275 16.32 0.280 34.871 1.000 15.68 ANISOU 1895 CB VAL 275 14.227 -0.004 32.483 1.000 16.05 ANISOU 1895 CB VAL 275 14.227 -0.004 32.483 1.000 16.05 ANISOU 1895 CB VAL 275 14.080 -1.186 33.426 1.000 17.04 ANISOU 1896 CG1 VAL 275 2045 1688 2740 -211 230 1 5 ANISOU 1897 CG2 VAL 275 12.847 0.608 32.203 1.000 18.45 ANISOU 1897 CG2 VAL 275 12.847 0.608 32.203 1.000 18.45 ANISOU 1897 CG2 VAL 275 1650 2412 292 8 -577 135 26 9 ANISOU 1898 N PRO 276 17.447 0.093 32.844 1.000 16.21 30 ANISOU 1898 N PRO 276 17.347 0.093 32.844 1.000 16.21 30 ANISOU 1898 N PRO 276 18.707 -0.434 33.399 1.000 18.10 16.21 30 ANISOU 1899 CA PRO 276 18.707 -0.434 33.399 1.000 18.10 16.21 30 ANISOU 1900 C PRO 276 19.382 0.541 34.521 1.000 17.52 30 ANISOU 1900 C PRO 276 19.382 0.541 34.521 1.000 17.52 30 ANISOU 1900 C PRO 276 19.380 0.171 35.481 1.000 17.52 30 ANISOU 1900 C PRO 276 19.380 0.171 35.481 1.000 17.52 30 ANISOU 1900 C PRO 276 19.380 0.171 35.481 1.000 17.52 30 ANISOU 1900 C PRO 276 19.380 0.171 35.481 1.000 17.52 30 ANISOU 1900 C PRO 276 19.380 0.171 35.481 1.000 17.52 30 ANISOU 1900 C PRO 276 2053 2004 2687 3121 306 771 -249 ANISOU 1900 C PRO 276 2053 2004 2687 3121 306 771 -249 ANISOU 1900 C PRO 276 2053 2006 2004 2687 3121 306 771 -249 ANISOU 1900 C PRO 276 2053 2006 2004 2687 3121 306 771 -249 ANISOU 1900 C PRO 276 2053 2006 2004 2687 3121 306 771 -249 ANISOU 1900 C PRO 276 2053 2006 2004 2687 3121 306 771 -249 ANISOU 1900 C PRO 276 2053 2006 2004 2007 2009 ANISOU 1900 C PRO 276 2053 2006 2004 2009 ANISOU 1900 C PRO 276 2053 2006 2004 2009 ANISOU 1900 C PRO 276 2053 2006 2004 2009 ANISOU 1900 C PRO 276 277 2466 277 247 247 247 247 247 247 247 247 247						
ATOM 1894 O VAL 275 16.623 0.280 34.871 1.000 15.68 8 ANISOU 1894 O VAL 275 16.623 0.280 34.871 1.000 15.68 8 ANISOU 1895 CB VAL 275 14.227 16.623 1655 2267 6 297 1 9 6 ANISOU 1895 CB VAL 275 16.35 1708 2755 -76 405 2 1 ANISOU 1895 CB VAL 275 16.35 1708 2755 -76 405 2 1 ANISOU 1896 CG1 VAL 275 14.080 1-1.186 3.425 1.000 17.04 ANISOU 1897 CG2 VAL 275 12.847 0.608 2.203 1.000 18.45 ANISOU 1897 CG2 VAL 275 16.50 242 2928 -57 135 2 6 9 ANISOU 1899 CG1 VAL 275 16.50 242 2928 -57 135 2 6 9 ANISOU 1899 CG2 VAL 275 16.50 242 2928 -57 135 2 6 9 ANISOU 1899 CG2 VAL 275 16.50 242 2928 -57 135 2 6 9 ANISOU 1899 CA PRO 276 19.382 0.541 33.399 1.000 18.10 2 ANISOU 1899 CA PRO 276 19.983 0.541 33.399 1.000 18.10 2 ANISOU 1900 C PRO 276 19.983 0.541 33.399 1.000 18.10 2 ANISOU 1900 C PRO 276 19.982 0.541 34.321 1.000 17.04 2 ANISOU 1900 C PRO 276 19.983 0.171 35.348 1.000 16.5 2 ANISOU 1903 CG PRO 276 19.590 0.796 3.214 3.21 1.000 17.06 2 ANISOU 1903 CG PRO 276 2015 2409 3047 24 280 46 8 ANISOU 1903 CG PRO 276 2053 206 264 267 3121 306 771 -249 ANISOU 1904 CD PRO 276 2053 206 264 267 3121 306 771 -249 ANISOU 1904 CD PRO 276 2053 206 2546 17.346 207 ANISOU 1905 N LEU 277 19.325 1.845 30.25 2.204 1.000 17.30 2.88 ANISOU 1906 CA LEU 277 19.932 2.204 1.000 19.83 2.204 ANISOU 1906 CA LEU 277 19.932 2.204 1.000 19.83 2.204 ANISOU 1907 C LEU 277 19.932 2.204 1.000 19.83 2.204 ANISOU 1908 CA LEU 277 20.950 2.204 1.000 19.83 2.204 ANISOU 1908 CA LEU 277 20.950 2.204 2.20				0.445	33.659	1.000 15.33
ANISOU 1894 O VAL 275 16.623 0.280 34.871 1.000 15.68 ANISOU 1895 CB VAL 275 14.227 -0.004 32.483 1.000 16.05 ATOM 1895 CB VAL 275 16.55 1708 27.55 -76 405 2 1 ATOM 1895 CG VAL 275 16.55 1708 27.55 -76 405 2 1 ATOM 1896 CG1 VAL 275 16.50 1708 27.55 -76 405 2 1 ATOM 1896 CG1 VAL 275 12.847 0.608 32.203 1.000 17.04 ANISOU 1897 CG2 VAL 275 16.50 245 16.88 27.40 -2.11 230 1 5 ATOM 1897 CG2 VAL 275 16.50 245 2 2432 2288 -57 135 2 6 9 ATOM 1898 N PRO 276 19.27 1700 2432 2288 -57 135 2 6 9 ATOM 1898 N PRO 276 19.27 1700 2532 97 589 3 6 9 ATOM 1899 CA PRO 276 19.382 0.541 30.25 14.7 616 -9 ATOM 1900 C PRO 276 19.982 19.61 34.321 1.000 18.10 ATOM 1900 C PRO 276 19.982 19.61 34.321 1.000 19.66 3 ATOM 19.01 O PRO 276 20.55 20.59 12.214 1.000 19.66 3 ATOM 19.02 CB PRO 276 18.852 -0.390 30.47 24.280 46.8 ATOM 19.03 CG PRO 276 18.852 -0.390 30.46 34.000 19.66 3 ATOM 19.04 CD PRO 276 20.51 30.98 1.000 19.66 3 ATOM 19.05 CD PRO 276 20.51 30.98 1.000 19.66 3 ATOM 19.05 CD PRO 276 20.51 30.98 1.000 19.66 3 ATOM 19.05 CD PRO 276 20.51 30.98 1.000 19.60 2.22 4 2.80 4.68 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 4.68 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 4.68 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 4.68 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 4.68 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 4.68 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 4.68 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 4.68 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 4.68 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 4.80 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 4 3.80 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 ATOM 19.05 CD PRO 276 20.51 30.98 30.46 34.00 20.22 4 2.80 ATOM 19.05 CD PRO 276 20.51 30.50 ATOM 19.05 CD PRO 276 20				1881	2139	116 392 - 45
ANISOU 1894 O VAL 275 14.227 -0.004 32.483 1.000 16 0.5 ANISOU 1895 CB VAL 275 16.35 -10.004 18.95 CB VAL 275 16.35 -10.004 18.95 CB VAL 275 16.35 -10.004 18.96 CG1 VAL 275 14.080 -1.18.6 3.3.42.6 1.000 16.0 5 ANISOU 18.96 CG1 VAL 275 12.847 0.608 2740 -211 230 1.5 ANISOU 18.97 CG2 VAL 275 16.50 -0.608 2740 -211 230 1.5 ANISOU 18.97 CG2 VAL 275 16.50 -0.608 2740 -211 230 1.5 ANISOU 18.98 N PRO 276 17.437 0.608 272.22 3 1.000 18.45 ANISOU 18.99 CA PRO 276 17.437 0.0093 32.844 1.000 16.21 ANISOU 18.99 CA PRO 276 17.35 2.15 ANISOU 18.99 CA PRO 276 17.35 2.15 ANISOU 19.00 C PRO 276 19.98 19.61 ANISOU 19.00 C PRO 276 19.98 19.61 ANISOU 19.01 O PRO 276 19.98 19.61 ANISOU 19.01 O PRO 276 19.98 19.61 ANISOU 19.02 CB PRO 276 19.98 19.61 ANISOU 19.02 CB PRO 276 19.590 -0.796 32.214 1.000 17.52 ANISOU 19.02 CB PRO 276 17.446 -0.021 ANISOU 19.03 CG PRO 276 17.446 -0.021 ANISOU 19.04 CD PRO 276 17.57 19.52 ANISOU 19.04 CD PRO 276 17.57 19.52 ANISOU 19.04 CD PRO 276 17.57 19.52 ANISOU 19.05 N EZU 277 19.52 1.845 ANISOU 19.06 CA EZU 277 19.962 ANISOU 19.07 C EZU 277 19.962 ANISOU 19.06 CA EZU 277 19.962 ANISOU 19.07 C EZU 277 19.962 ANISOU 19.00 CB EZU 277 20.994 AN		VAL	275 16.623	0.280	34.871	1.000 15.68
ANISOU 1895 CB VAL			275 2037		2267	
ANISOU 1895 CB VAL 275 1635 1708 2755 -76 405 2 1 ACROM 1896 CG1 VAL 275 14.080 16.83 3.426 1.000 17.04 ANISOU 1897 CG2 VAL 275 12.847 0.608 32.020 1.000 18.01 5 ANISOU 1897 CG2 VAL 275 1650 2432 2928 -57 135 26 9 ANISOU 1898 N PRO 276 17.437 0.093 32.844 1.000 16.21 ANISOU 1898 N PRO 276 19.27 1700 2532 97 589 3 6 ANISOU 1899 CA PRO 276 19.27 1700 2532 97 589 3 6 ANISOU 1890 C PRO 276 19.382 0.541 34.321 1.000 17.52 ANISOU 1900 C PRO 276 19.382 0.541 34.321 1.000 17.52 ANISOU 1900 C PRO 276 19.98 1961 297 30.99 1.000 17.52 ANISOU 1900 C PRO 276 19.590 ANISOU 1902 CB PRO 276 2015 2409 347 24.280 46.8 ANISOU 1902 CB PRO 276 2051 3098 3046 340 802 -288 ANISOU 1903 CG PRO 276 2051 3098 3046 340 802 -288 ANISOU 1903 CG PRO 276 2051 3098 3046 340 802 -288 ANISOU 1903 CG PRO 276 2051 3098 3046 340 802 -288 ANISOU 1903 CG PRO 276 2051 3098 3046 340 802 -288 ANISOU 1903 CG PRO 276 2051 3098 3046 340 802 -288 ANISOU 1903 CG PRO 276 2051 3098 3046 340 802 -288 ANISOU 1903 CG PRO 276 2051 3098 3046 340 802 -288 ANISOU 1903 CG PRO 276 2051 3098 3046 340 802 -288 ANISOU 1903 CG PRO 276 2051 3098 3046 340 802 -288 ANISOU 1905 N LEU 277 19.325 1885 3049 1.000 21.57 ANISOU 1905 CA LEU 277 19.9325 2306 2546 179 832 -311 8 ANISOU 1905 CA LEU 277 2035 2141 3171 -219 218 26 2 ANISOU 1906 CA LEU 277 2035 2141 3171 -219 218 26 2 ANISOU 1906 CA LEU 277 2035 2141 3171 -219 218 26 2 ANISOU 1908 CA LEU 277 2036 2367 3121 1.000 19.29 ANISOU 1908 CA LEU 277 2039 2011 388 14.22 87 ANISOU 1910 CG LEU 277 3764 3171 518 -487 -2057 85 3 ANISOU 1910 CG LEU 277 3764 3171 518 -487 -2010 17.00			275 14.227			
ATOM 1896 CG1 VAL 275 14.080 -1.186 33.426 1.000 17.04 ANISOU 1897 CG2 VAL 275 12.847 0.608 32.203 1.000 18.05 15 ATOM 1897 CG2 VAL 275 12.847 0.608 32.203 1.000 18.45 5 ATOM 1897 CG2 VAL 275 1650 2432 2928 -57 135 26 9 ATOM 1898 N PRO 276 17.437 0.093 32.844 1.000 16.21 ATOM 1899 CA PRO 276 18.707 -0.434 33.399 1.000 18.10 ANISOU 1893 N PRO 276 19.376 2115 30.25 147 616 -9 ATOM 1899 CA PRO 276 19.382 0.541 34.321 1.000 17.52 ANISOU 1900 C PRO 276 19.382 0.541 34.321 1.000 17.52 ANISOU 1901 O PRO 276 19.986 1.051 34.321 1.000 17.52 ANISOU 1901 O PRO 276 19.986 1.011 35.348 1.000 19.66 ANISOU 1902 CB PRO 276 19.986 1.011 35.348 1.000 19.66 ANISOU 1902 CB PRO 276 19.596 1.011 35.348 1.000 19.66 ANISOU 1903 CG PRO 276 2094 2687 3121 306 771 -249 ANISOU 1903 CG PRO 276 2051 3098 30.999 1.000 21.41 0.000 27.09 ANISOU 1904 CD PRO 276 2053 2.0061 31.368 1.000 18.17 ANISOU 1904 CD PRO 276 2053 2.0061 31.368 1.000 18.17 ANISOU 1905 N LEU 277 19.325 1.845 36.027 1.000 17.09 ANISOU 1905 CA LEU 277 19.962 21.845 36.249 1.000 19.34 ANISOU 1906 CA LEU 277 19.962 21.845 36.249 1.000 19.34 ANISOU 1906 CA LEU 277 19.815 2.957 37.319 1.000 19.34 ANISOU 1908 C LEU 277 19.815 2.957 37.319 1.000 19.29 ANISOU 1908 C LEU 277 2035 2141 3171 -219 218 26 2 ANISOU 1908 C LEU 277 2035 2141 3171 -219 218 26 2 ANISOU 1908 C LEU 277 2035 2141 3171 -219 218 26 2 ANISOU 1908 C LEU 277 2035 2141 3171 -219 218 26 2 ANISOU 1908 C LEU 277 2739 2011 3883 14 12 28 7 ANISOU 1910 C C LEU 277 2739 2011 3883 14 12 28 7 ANISOU 1910 C C LEU 277 2739 2011 3883 14 12 28 7 ANISOU 1910 C C LEU 277 273 362 230 511 1 0.00 31 0.4 ANISOU 1910 C C LEU 277 273 362 230 511 1 0.00 31 0.4 ANISOU 1910 C C LEU 277 273 362 230 511 1 0.00 31 0.4 ANISOU 1910 C C LEU 277 273 362 230 51 1 0.00 31 0.4 ANISOU 1910 C C LEU 277 273 362 230 51 1 0.00 31 0.4 ANISOU 1910 C C LEU 277 273 362 230 51 1 0.00 31 0.4 ANISOU 1910 C C LEU 277 273 362 364 374 374 374 374 374 374 374 374 374 37			275 1635		2755	
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ANISOU 1910 CG LEU 277 3662 2367 3978 -980 -547 9 4 4 ATOM 1911 CD1 LEU 277 22.396 4.839 35.069 1.000 38.04 ANISOU 1912 CD2 LEU 277 3764 3171 -487 -2057 8 5 3 ATOM 1912 CD2 LEU 277 4023 2018 6109 -366 508 7 3 2 ATOM 1913 N ALA 278 17.875 2.711 36.202 1.000 17.30 ANISOU 1913 N ALA 278 2015 1766 2793 74 218 1 1 5 ATOM 1914 CA ALA 278 17.124 2.712 37.464 1.000 16.75 ANISOU 1914 CA ALA 278 17.575 1.523 38.313 1.000 16.31 ANISOU 1915 C ALA 278 17.575 1.523 38.313 1.000 16.31 ANISOU 1915 C ALA 278 1849 1553 2794 -337 -196 1 0 7 ATOM 1916 O ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 1963 1839 2754 -62 -53 2 0 5 ANISOU 1918 N ARG 279 17.724 0.362 37.177 1.000 17.55 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ANISOU 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -7726 -1700 2 6 0 3			277 20.910	5.192		1.000 26.34
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ATOM 1912 CD2 LEU 277 3764 3171 7518 -487 -2057 853 ATOM 1912 CD2 LEU 277 4023 2018 6109 -366 508 7 3 2 ATOM 1913 N ALA 278 17.875 2.711 36.202 1.000 17.30 ANISOU 1913 N ALA 278 2015 1766 2793 74 218 1 1 5 ATOM 1914 CA ALA 278 17.124 2.712 37.464 1.000 16.75 ANISOU 1915 C ALA 278 17.575 1.523 38.313 1.000 16.31 ATOM 1915 C ALA 278 17.575 1.523 38.313 1.000 16.31 ANISOU 1915 C ALA 278 1849 1553 2794 -337 -196 1 0 7 ANISOU 1916 O ALA 278 17.718 1.635 39.523 1.000 17.26 ANISOU 1916 O ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 1963 1839 2754 -62 -53 2 0 5 ANISOU 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 - 1 1 ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 3 3.04 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 3 3.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2 6 0 3		1 LEU	277 22.396			
ATOM 1912 CD2 LEU 277 20.708 6.607 34.631 1.000 31.98 ANISOU 1912 CD2 LEU 277 4023 2018 6109 -366 508 7 3 2 ATOM 1913 N ALA 278 17.875 2.711 36.202 1.000 17.30 ANISOU 1913 N ALA 278 2015 1766 2793 74 218 1 1 5 ATOM 1914 CA ALA 278 17.124 2.712 ANISOU 1915 C ALA 278 2200 1566 2600 216 146 - 2 ATOM 1915 C ALA 278 17.575 1.523 38.313 1.000 16.31 ANISOU 1915 C ALA 278 1849 1553 2794 -337 -196 1 0 7 ATOM 1916 O ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 - 1 1 ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 2322 37.344 31.000 16.93 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ANISOU 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603			277 3764	3171	7518	
ATOM 1913 N ALA 278 17.875 2.711 36.202 1.000 17.30 ANISOU 1913 N ALA 278 17.124 2.712 37.464 1.000 16.75 ATOM 1914 CA ALA 278 2200 1566 2600 216 146 - 2 ATOM 1915 C ALA 278 17.575 1.523 38.313 1.000 16.31 ANISOU 1915 C ALA 278 17.7575 1.523 38.313 1.000 16.31 ANISOU 1916 O ALA 278 17.718 1.635 39.523 1.000 17.26 ANISOU 1916 O ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 - 1 1 ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ANISOU 1921 O ARG 279 19.687 -0.587 39.098 1.000 19.87 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603	ATOM 1912 CD		277 20.708	6.607	34.631	1.000 31.98
ATOM 1913 N ALA 278 17.875 2.711 36.202 1.000 17.30 ANISOU 1913 N ALA 278 2015 1766 2793 74 218 1 1 5 ATOM 1914 CA ALA 278 17.124 2.712 37.464 1.000 16.75 ANISOU 1915 C ALA 278 17.575 1.523 38.313 1.000 16.31 ANISOU 1915 C ALA 278 1849 1553 2794 -337 -196 1 0 7 ATOM 1916 O ALA 278 17.718 1.635 39.523 1.000 17.26 ANISOU 1916 O ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 1963 1839 2754 -62 -53 2 0 5 ANISOU 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 - 1 1 ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603	ANISOU 1912 CD			2018		
ATOM 1914 CA ALA 278 17.124 2.712 37.464 1.000 16.75 ATOM 1914 CA ALA 278 2200 1566 2600 216 146 - 2 ATOM 1915 C ALA 278 17.575 1.523 38.313 1.000 16.31 ANISOU 1915 C ALA 278 1849 1553 2794 -337 -196 1 0 7 ANISOU 1916 O ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 - 1 1 ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603	ATOM 1913 N				36.202	1.000 17.30
ATOM 1914 CA ALA 278 17.124 2.712 37.464 1.000 16.75 ANISOU 1914 CA ALA 278 2200 1566 2600 216 146 - 2 ATOM 1915 C ALA 278 17.575 1.523 38.313 1.000 16.31 ANISOU 1915 C ALA 278 1849 1553 2794 -337 -196 1 0 7 ATOM 1916 O ALA 278 17.718 1.635 39.523 1.000 17.26 ANISOU 1916 O ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 - 1 1 ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603				1766	2793	74 218 1 1 5
ATOM 1915 C ALA 278 17.575 1.523 38.313 1.000 16.31 ANISOU 1915 C ALA 278 1849 1553 2794 -337 -196 1 0 7 ATOM 1916 O ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 - 1 1 ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 2322 1399 2766 -178 26 3 0 8 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ANISOU 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 26 0 3			278 17.124		37.464	1.000 16.75
ATOM 1915 C ALA 278 17.575 1.523 38.313 1.000 16.31 ANISOU 1916 O ALA 278 17.718 1.635 39.523 1.000 17.26 ANISOU 1916 O ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 - 1 1 ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603					2600	216 146 - 2
ATOM 1916 O ALA 278 1849 1553 2794 -337 -196 1 0 7 ANISOU 1916 O ALA 278 1963 1839 2754 -62 -53 2 0 5 ATOM 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 - 1 1 ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603		ALA	278 17.575		38.313	1.000 16.31
ANISOU 1916 O ALA 278 1963 1839 2754 -62 -53 205 ATOM 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 - 1 1 ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603				1553	2794	-337 -196 1 0 7
ATOM 1917 CB ALA 278 1963 1839 2754 -62 -53 2 0 5 ANISOU 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603					39.523	1.000 17.26
ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 - 1 1 ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603					2754	-62 -53 2 0 5
ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603					37.177	1.000 17.55
ATOM 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 ANISOU 1918 N ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603			278 2109		2679	295 195 - 11
ATOM 1919 CA ARG 279 2322 1399 2766 -178 26 3 0 8 ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603	ALOM TATA N		279 17.724		37.696	1.000 17.07
ATOM 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603					2766	-178 26 3 0 8
ATOM 1920 C ARG 279 2377 1734 2323 15 -241 2 0 3 ATOM 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603			279 18.099		38.473	1.000 16.93
ATOM 1920 C ARG 279 19.477 -0.587 39.098 1.000 19.87 ANISOU 1920 C ARG 279 2491 2292 2766 -487 -384 5 4 3 ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603		-			2323	15 -241 203
ATOM 1921 O ARG 279 2491 2292 2766 -487 -384 5 4 3 ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603					39.098	
ATOM 1921 O ARG 279 19.687 -0.974 40.234 1.000 33.04 ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603					2766	-487 -384 5 4 3
ANISOU 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603			279 19.687		40.234	1.000 33.04
AIOM 1922 CB ARG 279 18.164 -2.042 37.517 1.000 20.04					4115	-1726 -1700 2603
	ATUM 1922 CE	ARG	279 18.164	-2.042	37.517	1.000 20.04

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- 76 -
                   ANISOU 1922 CB
                                                                                                                                                    ARG 279 2042 1609 3964 108 221 - ARG 279 16.742 -2.491 37.179 1.000 20.73
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                <u>--221 - 305</u>
                                                                               1923 CG
                   ANISOU 1923 CG
                                                                                                                                                                                                   279 2152 2728 2997 -98 -401 - 279 16.601 -3.422 35.990 1.000 24.81
                                                                                                                                                      ARG
                                                                                                                                                                                                                                                                                                                                                                                                                               -98 -401 -351
ANTSOU 1924 CD ARG 279 16.601 -3.422 35.990 1.000 24.81 ANTSOU 1925 NE ARG 279 17.575 -4.484 36.195 1.000 27.50 ANTSOU 1925 NE ARG 279 47.301 -5.725 36.620 1.000 41.33 ATOM 1926 CZ ARG 279 17.301 -5.725 36.620 1.000 41.33 ATOM 1927 NH1 ARG 279 16.024 -6.012 36.866 1.000 40.53 ATOM 1928 NH2 ARG 279 18.200 -6.688 36.807 1.000 53.27 ATOM 1928 NH2 ARG 279 18.200 -6.688 36.807 1.000 53.27 ATOM 1929 N GLU 280 220.390 0.119 ANTSOU 1929 N GLU 280 220.390 0.119 ANTSOU 1929 N GLU 280 21.72 276 ANTSOU 1930 CA GLU 280 21.72 276 ANTSOU 1931 C GLU 280 21.705 1.257 ANTSOU 1931 C GLU 280 2334 1968 3552 -281 285 2 0 ANTSOU 1931 C GLU 280 22.723 1.079 ANTSOU 1931 C GLU 280 22.723 1.079 ANTSOU 1931 C GLU 280 22.723 1.079 ANTSOU 1933 CB GLU 280 22.784 ATOM 1933 CB GLU 280 22.997 ANTSOU 1933 CB GLU 280 22.997 ANTSOU 1935 CD GLU 280 22.997 ANTSOU 1936 CE GLU 280 23.815 ANTSOU 1936 CE GLU 280 24.561 ANTSOU 1936 CE GLU 280 24.561 ANTSOU 1936 CE GLU 280 24.561 ANTSOU 1937 OEZ GLU 280 24.561 ANTSOU 1937 OEZ GLU 280 24.561 ANTSOU 1938 N CYS 281 20.877 ANTSOU 1938 N CYS 281 20.877 ANTSOU 1938 N CYS 281 20.881 20.881 20.881 20.897 ANTSOU 1938 N CYS 281 20.881 20.881 20.899 ANTSOU 1938 N CYS 281 20.881 20.881 20.882 20.899 ANTSOU 1938 N CYS 281 20.881 20.882 20.899 ANTSOU 1938 N CYS 281 20.881 20.882 20.899 ANTSOU 1938 S CYS 281 20.881 20.882 20.899 ANTSOU 1938 CYS 281 20.881 20.882 20.899 ANTSOU 1938 N CYS 281 20.881 20.882 20.882 20.899 ANTSOU 1938 N CYS 281 20.881 20.882 20.882 20.899 ANTSOU 1938 N CYS 281 20.881 20.882 20.882 20.899 ANTSOU 1938 N CYS 281 20.881 20.882 20.882 20.899 ANTSOU 1938 N CYS 281 20.882 20.882 20.899 ANTSOU 1938 CO CYS 281 20.882 20.899 ANTSOU 1938 CO CYS 281 20.899 ANTSOU 1938 CO CYS 281 20.899 ANTSOU 1934 CG CYS 281 
                                                                               1924 CD
                   MOTA
                                                                                                                                                      ARG
                   ANISOU 1924 CD
                                                                                                                                                                                               279 3213 2982 3231 -1 -507 -609
279 17.575 -4.484 36.195 1.000 27.50
                                                                                                                                                      ARG
 ATOM 1945 CA GLY 282 18.675 0.750 43.744 1.000 17.07

ATOM 1946 C GLY 282 17.194 0.496 43.538 1.000 14.91

ATOM 1946 C GLY 282 1601 1645 2417 -135 -453 3 7 8

ANISOU 1947 O GLY 282 160.480 -0.062 44.380 1.000 16.38

ATOM 1948 N PHE 283 16.625 0.919 42.404 1.000 13.44

ATOM 1948 N PHE 283 1563 1539 2006 -189 -336 -115

ANISOU 1949 CA PHE 283 15.173 0.829 42.203 1.000 14.52

ATOM 1950 C PHE 283 15.17 0.829 42.203 1.000 14.52

ATOM 1950 C PHE 283 15.19 1314 2137 -121 -338 174

ANISOU 1950 C PHE 283 15.311 -1.184 40.837 1.000 13.08

ATOM 1951 O PHE 283 1366 1418 2578 -142 -78 1 7

ANISOU 1952 CB PHE 283 14.749 1.800 41.078 1.000 13.76

ANISOU 1952 CB PHE 283 1814 1288 2125 -39 -268 0
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- 78 -
 ANISOU 1983 O
                 LEU 287 1885
                                 2275
                                         2645
                                                109
                                                      300 - 275
 MOTA
        1984 CB LEU
                      287 9.954
                                 -1.480 34.118 1.000 14.37
 ANISOU 1984 CB
                LEU
                      287 1773 • 1380
                                         2306
                                                -34
                                                      248 107
 ATOM
        1985 CG
                LEU
                      287 9.362
                                 -0.603 35.231 1.000 \overline{14}.32
 ANISOU 1985 CG LEU
                      287 1421
                                 1496
                                         2523
                                                62 52 - 1 5 8
 ATOM
        1986 CD1 LEU
                      287 10.143 0.705
                                         35.413 1.000 14.53
 ANISOU 1986 CD1 LEU
                     287 1672
                                 1444
                                         2403
                                                0
                                                   -146 143
        1987 CD2 LEU
 ATOM
                     287 7.921
                                 -0.197
                                         34.820 1.000 16.03
 ANISOU 1987 CD2 LEU
                     287 1476
                                 2035
                                         2579
                                                166
 ATOM
        1988 N
                                                      -100 - 7
                 ASP
                     288 9.256
                                 -4.060
                                         31.958 1.000 15.09
 ANISOU 1988 N
                ASP
                     288 2041
                                 1611
                                         2081
                                                73 175 - 216
        1989 CA
 ATOM
                ASP
                     288 9.764
                                -4.722
                                         30.757 1.000 16.55
 ANISOU 1989 CA ASP
                     288 1992
                                 2028
                                         2268
                                                29 335 - 314
 MOTA
        1990 C
                ASP
                     288 10.437 -3.682
                                         29.874 1.000 18.74
 ANISOU 1990 C
                ASP
                     288 2484 2597
                                         2040
                                                -231
                                                      97 8 1
 ATOM
        1991 0
                ASP
                     288 9.998
                               -2.526
                                         29.849 1.000 25.48
 ANISOU 1991 O
                     288 3382 2433
288 8.659 -5.49
                ASP
                                         3865
                                               -322
 ATOM
        1992 CB
                                                      639 346
                ASP
                                -5.490
                                        30.060 1.000 19.23
 ANISOU 1992 CB
                ASP
                     288 2431
                                 2414
                                         2460
                                               -209
 ATOM
        1993 CG ASP
                                                      258
                     288 9.139
                                 -6.468
                                        29.000 1.000 19.50
 ANISOU 1993 CG ASP
                     288 2688
                                 2223
                                         2499
                                               -49
        1994 OD1 ASP
                     288 10.173 -7.145
                                                      393 - 552
ATOM
                                        29.185 1.000 27.03
ANISOU 1994 OD1 ASP
                     288 3134
                                3038
                                        4100
                                               624
ATOM
        1995 OD2 ASP
                                                      427 - 716
                     288 8.458
                                -6.566
                                        27.955 1.000 31.00
ANISOU 1995 OD2 ASP
                     288 3596
                                4859
                                        3325
                                               307
ATOM
                                                     -361 - 2100
        1996 N
                    289 11.489 -4.035
                GLY
                                        29.137 1.000 22.68
ANISOU 1996 N
                GLY
                     289 2960
                                2893
                                        2765
                                               -531 778 116
       1997 CA GLY
                     289 12.008 -3.083 28.169 1.000 25.60
ANISOU 1997 CA GLY
                     289 3678
                                3562
                                        2486
                                               -1469 558 1 1
       1998 C
ATOM
                     289 12.988 -2.078 28.725 1.000 21.08
                GLY
ANISOU 1998 C
                GLY
                     289 2567 2916 2528 -485 353 150
289 13.411 -2.097 29.891 1.000 23.72
                     289 2567
ATOM
       1999 O
                GLY
ANISOU 1999 O
               GLY
                     289 3428
                                3219
                                        2364
                                               -1104 440 113
ATOM
       2000 N
               GLU
                     290 13.402 -1.168 27.818 1.000 18.32
ANISOU 2000 N
               GLU
                     290 2246
                                2396
                                        2319
                                               -145 616 -115
ATOM
       2001 CA GLU
                     290 14.538 -0.301 28.074 1.000 17.75
ANISOU 2001 CA GLU
                    290 1912 2419
290 14.261 1.058
                     290 1912
                                        2412
                                               97 770 - 367
       2002 C
MOTA
               GLU
                                        28.696 1.000 17.90
ANISOU 2002 C
               GLU
                    290 2180
                                2308
                                        2313
                                               50 711 - 297
ATOM
       2003 0
               GLU
                    290 15.143 1.619
                                        29.353 1.000 17.58
ANISOU 2003 O
               GLU
                    290 2525
                                2050
                                        2104
ATOM
                                             -35
                                                     380 165
       2004 CB
               GLU
                    290 15.341
                               -0.161
                                       26.785 1.000 23.21
ANISOU 2004 CB
               GLU
                    290 3184
                                2508
                                        3126
                                               -273 1753 -467
ATOM
       2005 CG
               GLU
                    290 15.833 -1.492
ANISOU 2005 CG
                                        26.226 1.000 24.55
               GLU
                    290 3609
                                2992
                                        2725
                                               348
ATOM
                                                     1232 - 743
       2006 CD
               GLU
                    290 16.676 -2.280
                                        27.221 1.000 30.03
ANISOU 2006 CD
               GLU
                    290 3365
                                3708
                                        4337
                                               476
       2007 OE1 GLU
ATOM
                                                     753 -211
                    290 17.492 -1.684
                                        27.947 1.000 40.04
ANISOU 2007 OE1 GLU
                    290 5043
                               6674
                                        3498
ATOM
                                               525
                                                     36 - 1226
       2008 OE2 GLU
                    290 16.622 -3.527 27.237 1.000 51.76
ANISOU 2008 OE2 GLU
                    290 8785
                                3812
                                        7070
                                               -12
                                                     -483 1583
ATOM
       2009 N
               THR
                    291 13.064 1.578
                                        28.486 1.000 18.14
ANISOU 2009 N
               THR
                    291 2305
                                2486
                                        2103 224
ATOM
                                                     711 - 321
       2010 CA
               THR
                    291 12.697 2.896
                                        29.049 1.000 18.72
ANISOU 2010 CA
               THR
                    291 2521
                                2080
                                        2511
                                               105
ATOM
                                                     1131 6 6
       2011 C
                    291 11.278 2.744
               THR
                                        29.593 1.000 15.79
ANISOU 2011 C
               THR
                    291 2178
                                1758
                                        2064
                                               134
                                                     538 - 50
MOTA
       2012 0
               THR
                    291 10.517 1.834
                                        29.217 1.000 18.62
ANISOU 2012 O
               THR
                    291 2764
                                1966
                                        2344 - 248
ATOM
       2013 CB
                                                     664 - 311
               THR
                    291 12.722 4.031
                                        28.044 1.000 21.54
ANISOU 2013 CB
               THR
                    291 3043
                               2625
                                        2516
                                             -164
                                                     891
                                                          3 6 2
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- 79 -2014 OG1 THR 291 11.695 3.862 27.077 1.000 25.98 ATOM ANISOU 2014 OG1 THR 291 3160 27.292 1.000 24.20 291 3199 3832 2164 -445 930 5 3 3 292 10.959 3.658 30.492 1.000 14.84 292 1637 1656 2347 200 420 292 9.675 3.657 703 503 2015 CG2 THR ANISOU 2015 CG2 THR 2016 N ALA ANISOU 2016 N 1656 2347 200 429 -153 3.657 31.179 1.000 13.84 ALA 2017 CA ALA 292 9.675 MOTA ANISOU 2017 CA ALA 292 1488 ALA 292 1488 1477 2294 170 299 7 8 ALA 292 9.356 5.065 31.619 1.000 12.65 2018 C ATOM ALA 292 1334 1564 1908 60 144 - 139 ALA 292 10.228 5.939 31.710 1.000 14.27 ALA 292 1529 1596 2295 -35 109 1 ANISOU 2018 C 2019 0 ATOM ANISOU 2019 O 1596 2295 -35 109 1 1 6 2.754 32.414 1.000 14.02 2020 CB ALA 292 9.670 MOTA 1580 ANISOU 2020 CB ALA 292 1693 ATOM 2021 N THR 293 8.054 ANISOU 2021 N THR 293 1468 2053 37 22 - 27 31.916 1.000 13.54 5.258 1617 2021 N THR 293 1468 1617 2058 117 373 -118 2022 CA THR 293 7.605 6.546 32.424 1.000 13.40 ATOM ANISOU 2022 CA THR 293 1565 1647 1877 152 209 -232 ATOM 2023 C THR 293 7.407 6.482 33.952 1.000 12.09 ANISOU 2023 C THR 293 1345 1322 1927 -62 326 -12 ATOM 2024 O THR 293 7.214 5.441 34.555 1.000 12.93 1322 1927 -62 326 - 1 5.441 34.555 1.000 12.93 1356 2170 -190 194 9 0 ANISOU 2024 O THR 293 1385 7.058 31.788 1.000 13.45 2025 CB THR 293 6.295 2025 CB THR 293 1598 1579 1935 95 345 3 4 5 2026 OG1 THR 293 5.273 6.112 32.117 1.000 13.75 2026 OG1 THR 293 1672 1570 1981 -12 314 1 3 5 2027 CG2 THR 293 6.476 7.139 30.272 1.000 15.93 ANISOU 2025 CB THR ATOM 2026 OG1 THR ANISOU 2026 OG1 THR 293 1672 MOTA 293 2121 294 7.241 294 1607 ANISOU 2027 CG2 THR 2022 1911 255 434 337 7.661 34.544 1.000 12.81 2028 N MOTA PHE 1822 -83 149 -151 35.935 1.000 12.37 1899 -267 166 -289 ANISOU 2028 N PHE 1440 7.773 2029 CA PHE 294 6.857 ANISOU 2029 CA PHE 294 1332 1469 2030 C ATOM PHE 294 5.556 7.022 36.184 1.000 12.36 ANISOU 2030 C 1361 1999 -151 30 - 3 6 6.253 37.143 1.000 13.27 1410 2076 -191 183 4 6 9.271 36.267 1.000 13.83 PHE 294 1336 PHE 294 5.403 MOTA 2031 0 ANISOU 2031 O PHE 294 1556 MOTA 2032 CB PHE 294 6.698 ANISOU 2032 CB PHE 294 2039 ATOM 2033 CG PHE 294 6.306 ANISOU 2033 CG PHE 294 1786 1351 1866 -192 -29 -1 9.488 37.711 1.000 13.10 1866 -192 -29 -177 MOTA 2034 CD1 PHE 294 7.207 ANISOU 2034 CD1 PHE 294 2132 294 4.964 294 2156 294 6.810 2035 CD2 PHE ANISOU 2035 CD2 PHE 294 2156 2263 2575 565 332 5 7 294 6.810 9.608 40.054 1.00@ 17.72 294 2348 2296 2086 -308 -362 -136 294 4.591 10.010 39.324 1.000 19.37 2036 CE1 PHE MOTA ANISOU 2036 CE1 PHE 294 2348 MOTA 2037 CE2 PHE 294 2078 294 5.507 294 2443 ANISOU 2037 CE2 PHE 2541 2740 330 232 -630 9.956 40.355 1.000 18.36 2038 CZ PHE ATOM ANISOU 2038 CZ PHE 2855 -394 -55 -245 2039 N MOTA GLN ANISOU 2039 N GLN 295 3.320 295 1266 295 3.512 2040 CA GLN ATOM 6.484 35.408 1.000 12.76 ANISOU 2040 CA GLN 1215 2365 7 -157 -117 4.984 35.318 1.000 12.24 1256 1944 10 1 - 7 3 4.238 36.101 1.000 13.61 2041 C GLN ANISOU 2041 C GLN 295 1449 GLN 295 2.922 GLN 295 1323 GLN 295 2.375 GLN 295 1227 ATOM 2042 0 ANISOU 2042 O 1427 2424 7 85 1 5 5 6.975 34.317 1.000 14.31 2043 CB ATOM GLN ANISOU 2043 CB 1594 2616 81 -133 192 6.256 34.249 1.000 14.03 ATOM 2044 CG 295 1.062 GLN

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	2244		~			- 80 -		
ANISOU			GLN		1391	1509	2430	-59 -300 4 7
ATOM	2045		GLN	295	0.157	5.687		1.000 13.56
ANISOU			GLN		1305	1486	2361	133 -117 1 6 5
ATOM	2046				0.459	7.693		1.000 15.35
ANISOU	2046				1811	1651 6.026	2371	161 206 220
ATOM ANISOU					-0.982			1.000 15.04
ATOM	2047		ASP		1225	1995	2493	75 -139 - 9 9
ANISOU			ASP		4.363 1425	4.463		1.000 12.66
ATOM	2049		ASP		4.653	1396 3.016	1990	181 -112 - 110
ANISOU			ASP		1628	1274	1755	1.000 12.26
ATOM	2050		ASP		5.167	2.569		53 -51 -151 1.000 11.57
ANISOU			ASP		1199	1300	1895	-82 30 - 22
ATOM	2051		ASP		4.854	1.460		1.000 13.08
ANISOU			ASP		1534	1368	2070	-107 38 1 3 9
ATOM	2052		ASP		5.709	1368		1.000 14.18
ANISOU			ASP		1870	1700	1819	141 30 - 378
ATOM	2053		ASP		5.295	2.848	31.952	1.000 13.32
ANISOU	2053	CG	ASP		1655	1557	1848	-58 67 2
ATOM	2054	OD1	ASP		4.110	2.725		1.000 15.83
ANISOU					1680	1935	2402	-68 -126 -189
ATOM	2055	OD2	ASP		6.212	3.098	31.114	1.000 15.27
ANISOU					1757	1937	2106	-229 137 177
ATOM	2056		TRP		6.038	3.352		1.000 12.26
ANISOU			TRP		1325	1403	1931	-34 -123 -118
	2057		TRP		6.683	2.960		1.000 12.82
ANISOU			TRP		1328	1599	1943	-104 -49 151
ATOM ANISOU	2058		TRP		5.746	3.007		1.000 13.13
ANISOU	2059		TRP TRP		1418 5.565	1580		24 -23 1 8 5
ANISOU			TRP		1554	2.030 1619		1.000 14.03
ATOM	2060		TRP	297	7.908	3.847	2159	102 137 3 2 0 1.000 13.68
ANISOU			TRP		1130	1692	2376	-19 -169 1 5 1
ATOM	2061		TRP		8.646	3.455		1.000 13.28
ANISOU			TRP		1143	1646	2255	
ATOM	2062	CD1	TRP		8.932	2.179		1.000 15.58
ANISOU	2062	CD1	TRP		1615	1689	2618	275 -544 - 77
ATOM	2063				9.144	4.353	40.189	1.000 14.69
ANISOU	2063	CD2	TRP		1327	1693	2562	-117 -219 5
ATOM	2064	NE1	TRP		9.583	2.265		1.000 15.34
ANISOU					1378	1853	2598	70 -494 7 5
ATOM ANISOU	2065	CEZ	TRP	297	9.724	3.597		1.000 16.13
ATOM			TRP	297	1241 9.094	2009	2880	182 -676 - 196
ANISOU					3040	5.756 1658		1.000 22.13
ATOM			TRP	297	10.318	1 1 2 0		-665 £ -1408 129 1.000 18.45
ANISOU				297	2204	2387	2418	44 - 326 - 331
ATOM	2068				9.670	6.353		1.000 21.55
ANISOU				297	2916	2104	3167	-55 -752 - 458
ATOM	2069	CH2	TRP		10.258	5.546		1.000 23.53
ANISOU	2069	CH2	TRP		3298	2356	3285	-320 -1146 -344
ATOM	2070		ILE	298	5.106	4.167		1.000 13.58
ANISOU			ILE		1324	1726	2108	241 -167 1 2 7
ATOM	2071	CA	ILE		4.299	4.440	40.229	1.000 14.68
ANISOU			ILE		1413	2177	1986	-13 -161 - 208
ATOM	2072		ILE		2.841	4.054		1.000 12.02
ANISOU		C	ILE		1455	1300	1813	56 -239 402
ATOM ANISOU	2073		ILE		2.182	3.782		1.000 13.67
ATOM	2073	-	ILE		1732	1582	1881	-23 -4 1 9 3
ANISOU			ILE ILE		4.428 2261	5.914	40.673	1.000 19.45
141200	2014	CD	TUE	230	2 Z O I	2446	2683	-699 237 -835

	4-6				
					3,

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2075 CG1 ILE 298 5.907 MOTA 6.245 41.001 1.000 27.83 4275 6.319 3344 ANISOU 2075 CG1 ILE 298 2776 -1314 -556 -1030 3525 2076 CG2 ILE MOTA 298 3.679 41.929 1.000 25.05 ANISOU 2076 CG2 ILE 298 3770 2405 -57 255 - 983 5.628 42.306 1.000 43.32 2077 CD1 ILE 298 6.368 ANISOU 2077 CD1 ILE 298 4561 7224 4674 -652 -1890 3.980 38.893 1.000 12.16 4674 -652 -1890 -117 299 2.317 299 1432 2078 N GLYATOM ANISOU 2078 N 299 1432 1308 1879 78 -304 1 0 6 299 0.918 3.741 38.670 1.000 12.98 GLY2079 CA GLY MOTA 299 1276 1279 2379 106 -188 -1 299 0.135 5.017 38.378 1.000 13.09 ANISOU 2079 CA GLY 2379 106 -188 - 154 2080 C MOTA GLY
 299 1421
 1403
 2151
 113
 -231 1

 299 0.738
 6.025
 38.017 1.000 14.00

 299 1713
 1353
 2252
 122
 289

 300 -1.183
 4.917
 38.447 1.000 13.08
 ANISOU 2080 C GLY -231 1 1 8 2081 O GLYMOTA ANISOU 2081 O GLYATOM 2082 N ANISOU 2082 N GLYATOM 2082 N GLY 300 -1.183 4.917 38.447 1.000 13.08 ANISOU 2082 N GLY 300 1325 1545 2099 146 -267 -145 ATOM 2083 CA GLY 300 -2.075 5.966 37.992 1.000 13.45 ANISOU 2083 CA GLY 300 1447 1521 2143 116 -415 -143 ATOM 2084 C GLY 300 -2.519 6.972 39.042 1.000 12.94 ANISOU 2084 C GLY 300 1098 1365 2456 -52 -407 -192 GLY 300 1098 1365 2456 -52 -407 -GLY 300 -3.262 7.875 38.672 1.000 13.39 GLY 300 1321 1342 2423 130 ATOM 2085 O ANISOU 2085 O ATOM 2085 O GLY 300 -3.262 7.875 38.672 1.000 13.39

ANISOU 2085 O GLY 300 1321 1342 2423 -19 -217 - 4 5

ATOM 2086 N ASN 301 -1.973 6.845 40.254 1.000 13.35

ANISOU 2086 N ASN 301 1494 1429 2151 -225 -232 - 1 0 4

ATOM 2087 CA ASN 301 -2.162 7.842 41.313 1.000 13.83

ANISOU 2087 CA ASN 301 1590 1435 2230 -194 -38 - 6 1

ATOM 2088 C ASN 301 -0.837 8.254 41.885 1.000 12.46

ANISOU 2088 C ASN 301 1676 1268 1791 -35 -142 - 2 0

ATOM 2089 O ASN 301 -0.007 7.405 42.169 1.000 13.89

ANISOU 2089 O ASN 301 1831 1355 2093 73 -144 -1 3

ATOM 2090 CB ASN 301 -3.075 7.238 42 360 1.000 16 0.1 301 1831 1355 2093 73 -144 -13 301 -3.075 7.238 42.360 1.000 16.01 301 1632 1909 2542 77 200 5 ATOM 2090 CB ASN ANISOU 2090 CB ASN 2090 CB ASN 301 1632 1909 2542 77 224 3 1 5 2091 CG ASN 301 -3.942 8.199 43.106 1.000 18.23 2091 CG ASN 301 1986 2508 2435 190 152 -ATOM ANISOU 2091 CG ASN 2435 190 152 - 90 MOTA 2092 OD1 ASN 301 -4.973 8.690 42.614 1.000 17.44 ANISOU 2092 OD1 ASN 301 1606 1626 3394 -21 144 -190 ATOM 2093 ND2 ASN 301 -3.518 8.454 44.338 1.000 33.30 ANISOU 2093 ND2 ASN 301 2804 6923 2928 1012 -230 -1523 ATOM 2094 N TYR 302 -0.595 9.564 42.073 1.000 12.96 ATOM 2094 N TYR 302 -0.595 9.564 42.073 1.000 12.96
ANISOU 2094 N TYR 302 1662 1278 1985 -69 -21 -13
ATOM 2095 CA TYR 302 0.674 9.948 42.702 1.000 13.48
ANISOU 2095 CA TYR 302 1673 1259 2192 -130 -132 3 4
ATOM 2096 C TYR 302 0.768 9.269 44.078 1.000 12.63
ANISOU 2096 C TYR 302 1413 1293 2092 53 44 1 9
ATOM 2097 O TYR 302 -0.218 9.151 44.806 1.000 14.15
ANISOU 2097 O TYR 302 1332 1737 2305 -65 48 -27
ATOM 2098 CB TYR 302 0.764 11.472 42.916 1.000 13.30
ANISOU 2098 CB TYR 302 1635 1192 2226 -81 33 4 1
ATOM 2099 CG TYR 302 1.159 12.143 41.619 1.000 12.02
ANISOU 2099 CG TYR 302 1586 1103 1880 -59 -25 -27 -21 -135 302 1.133 12.143 41.613 1.000 12.02 302 1.586 1103 1880 -59 -25 -27 302 2.501 12.233 41.275 1.000 13.11 302 1633 1284 2066 -80 11 -18 302 0.235 12.709 40.739 1.000 12.52 302 1576 1132 2049 -44 13 -127 ANISOU 2099 CG TYR -25 -271 MOTA 2100 CD1 TYR ANISOU 2100 CD1 TYR 2101 CD2 TYR ANISOU 2101 CD2 TYR 2102 CE1 TYR ATOM 302 2.933 12.822 40.119 1.000 12.29 ANISOU 2102 CE1 TYR ATOM 2103 CE2 TYR 302 1581 1043 2045 -185 -84 - 7.7 302 0.637 13.273 39.535 1.000 14.12 302 1462 1443 2458 -241 15 3 2 5 ANISOU 2103 CE2 TYR 302 1462 1443 2458 -241 15 3 2 5 302 1.983 13.347 39.241 1.000 12.69* ATOM 2104 CZ TYR ANISOU 2104 CZ TYR 302 1483 1224 2113 -287 -91 1 0 MOTA 2105 OH TYR 302 2.376 13.866 38.013 1.000 13.42

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- 82 -ANISOU 2105 OH TYR 302 1505 1469 2124 -93 33 146 2106 N 303 1.956 44.450 1.000 13.92 VAL 8.855 MOTA ANISOU 2106 N VAL 303 1406 1637 2246 153 88 9 9 2107 CA VAL 8.336 45.746 1.000 14.51 303 2.355 ATOM ANISOU 2107 CA 303 1838 303 3.498 -137 -391 - 74 VAL 1320 2355 9.244 MOTA 2108 C VAL 46.239 1.000 15.23 ANISOU 2108 C VAL 303 1404 1507 2876 -102 -105 - 348 MOTA 2109 O VAL 303 4.471 9.386 45.512 1.000 18.70 303 1859 303 2.856 303 2140 1861 6.880 ANISOU 2109 O VAL 3386 -239 326 -504 MOTA 2110 CB VAL 45.632 1.000 16.75 2905 16 -759 -123 47.017 1.000 19.53 ANISOU 2110 CB VAL 1319 2111 CG1 VAL 303 3.279 6.401 MOTA ANISOU 2111 CG1 VAL 303 2185 1951 3284 232 -1054 148 303 1.723 303 2476 304 3.349 45.125 1.000 17.82 2112 CG2 VAL 5.956 MOTA ANISOU 2112 CG2 VAL 2852 -213 -558 - 406 1442 47.378 1.000 14.07 9.900 2113 N ATOM ASN ANISOU 2113 N ASN 304 1409 1369 2566 -39 -407 - 86 10.928 47.772 1.000 14.31 MOTA 2114 CA ASN 304 4.317 1387 10 304 1474 304 5.450 304 1360 1387 2578 -102 -424 - 5 5 10.397 48.637 1.000 13.75 1487 2378 34 -274 - 8 7 10.962 48.584 1.000 14.60 ANISOU 2114 CA ASN 2115 C MOTA ASN ANISOU 2115 C ASN MOTA 2116 0 ASN 304 6.539 304 1314 304 3.589 304 1710 ANISOU 2116 O ASN 1795 2438 -34 -55 -320 12.035 48.551 1.000 14.26 ASN 2117 CB ANISOU 2117 CB ASN 2494 6 -303 176 1214 12.661 47.642 1.000 14.81 304 2.535 MOTA 2118 CG ASN ANISOU 2118 CG ASN 304 1551 1627 2449 23 -114 402 13.255 46.622 1.000 16.52 MOTA 2119 OD1 ASN 304 2.866 304 1896 304 1.290 1746 2636 80 19 5 8 9 12.595 48.102 1.000 18.43 2980 2463 127 -10 1 9 9 9.413 49.463 1.000 16.36 ANISOU 2119 OD1 ASN 2120 ND2 ASN MOTA ANISOU 2120 ND2 ASN 304 1560 MOTA 2121 N ILE 305 5.175 305 1546 305 6.173 ANISOU 2121 N 1553 3117 -78 -503 2 6 6 ILE 50.407 1.000 14.85 8.890 1537 2122 CA ILE ANISOU 2122 CA ILE 305 1670 2436 165 -277 - 40 2123 C 305 6.183 7.372 50.352 1.000 15.78 ATOM ILE ANISOU 2123 C ILE 305 1527 1555 2914 95 -438 - 51 305 5.231 305 1463 305 5.949 6.736 49.886 1.000 17.54 ATOM 2124 0 ILE 3412 -131 -404 5 51.818 1.000 17.80 ANISOU 2124 O ILE 1789 9.430 2125 CB ILE ATOM ANISOU 2125 CB ILE 305 2167 1962 2634 -23 265 -209 305 4.578 9.091 52.416 1.000 18.93 2126 CG1 ILE MOTA ANISOU 2126 CG1 ILE ATOM 2127 CG2 ILE 305 1716 305 6.171 2948 2526 1 -218 -163 10.944 51.823 1.000 19.17 1863 2737 70 -534 -405 ANISOU 2127 CG2 ILE 305 2685 9.459 2128 CD1 ILE 305 4.415 53.863 1.000 21.28 305 2521 306 7.246 306 1738 306 7.424 ANISOU 2128 CD1 ILE 2902 2662 19 452 - 71 6.806 50.908 1.000 14.59 MOTA 2129 N ARG ANISOU 2129 N 1641 2165 52 -356 271 5.360 50.828 1.000 15.25 ARG 2130 CA ARG ATOM ANISOU 2130 CA ARG 306 1509 2622 139 -302 7 7 1663 4.903 1464 5.61 306 8.234 4.903 52.024 1.000 15.02 2131 C MOTA ARG 306 1588 306 9.141 306 1682 ANISOU 2131 C 1464 2656 133 -332 -5.614 52.433 1.000 16.63 2101 2536 -219 -294 -ARG -332 - 21 MOTA 2132 0 ARG ANISOU 2132 O -219 -294 -168 ARG 4.943 49.532 1.000 16.31 2133 CB ARG 306 8.135 -100 -270 -150 ANISOU 2133 CB ARG 306 1820 1681 2697 306 8.226 306 2476 306 8.401 MOTA 2134 CG ARG 3.414 49.377 1.000 18.43 ANISOU 2134 CG 2828 40 -194 -156 47.900 1.000 18.26 ARG 1700 ATOM 2135 CD ARG 3.068 ANISOU 2135 CD 306 2087 1971 2880 ARG -120 -145 -330

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- 83 -2136 NE MOTA ARG 306 7.136 3.228 47.188 1.000 20.53 ANISOU 2136 NE 306 2442 ARG 2013 3345 -577 -663 -234 MOTA 2137 CZ ARG 306 6.980 3.178 45.873 1.000 20.27 ANISOU 2137 CZ ARG 306 2330 2057 3316 3.73 -522 2 0 2138 NH1 ARG 306 8.086 45.107 1.000 22.13 3.000 ANISOU 2138 NH1 ARG 306 2136 2580 3695 274 -589 - 723 2139 NH2 ARG 306 5.759 3.250 45.341 1.000 18.44 ANISOU 2139 NH2 ARG 306 2107 1838 3062 259 -285 8 4 307 7.898 2140 N ARG 3.775 52.612 1.000 19.10 ANISOU 2140 N 307 2716 ARG 1872 2671 -294 -607 3 2 7 307 8.576 2141 CA ARG 53.768 1.000 21.13 3.212 ANISOU 2141 CA ARG 307 3321 2201 2504 -48 -845 1 3 9 MOTA 2142 C ARG 307 9.536 53.277 1.000 23.30 2.138 ANISOU 2142 C ARG 307 3417 2170 3267 -1046 3 9 181 2143 0 307 9.385 ATOM ARG 52.187 1.000 21.01 1.601 ANISOU 2143 O 307 2574 ARG 2355 3052 174 -728 1 1 2 MOTA 2144 CB ARG 307 7.557 2.522 54.694 1.000 27.30 ANISOU 2144 CB ARG 307 4545 3184 2645 -13 -247 7 0 5 2145 CG MOTA ARG 307 6.839 3.488 55.629 1.000 46.30 ANISOU 2145 CG ARG 307 6310 6374 4907 1655 - 970 215 2146 CD ATOM ARG 307 7.054 3.085 57.085 1.000 66.50 ANISOU 2146 CD ARG 307 11107 10355 3806 -2980 2792 -1145 2147 NE ATOM ARG 307 5.989 2.203 57.531 1.000 78.91 ANISOU 2147 NE ARG 307 11821 12833 5330 -4530 1969 - 5 2148 CZ ATOM ARG 307 5.987 1.285 58.479 1.000 73.67 ANISOU 2148 CZ ARG 307 7704 14382 5907 -4724 1249 1051 2149 NH1 ARG ATOM 307 7.063 1.038 59.214 1.000 80.32 ANISOU 2149 NH1 ARG 307 6613 17949 5955 -3290 2179 1 0 5 ATOM 2150 NH2 ARG 307 4.872 0.597 58.707 1.000 73.74 ANISOU 2150 NH2 ARG 307 9116 15919 2983 -6954 438 -917 308 10.551 1.861 ATOM 2151 N THR 54.113 1.000 25.61 ANISOU 2151 N THR 308 4234 2212 3285 536 -1421 -232 2152 CA THR 308 11.308 0.640 53.822 1.000 30.02 ANISOU 2152 CA THR 308 3468 1939 5998 225 -1629 - 1942153 C THR 308 10.468 -0.611 54.030 1.000 25.42 ANISOU 2153 C THR 308 2915 2190 4552 453 -626 - 321 2154 0 ATOM THR 308 9.523 -0.768 54.787 1.000 30.10 ANISOU 2154 O THR 308 4042 3482 3912 614 -217 -125 ATOM 2155 CB THR 308 12.581 0.531 54.688 1.000 26.09 ANISOU 2155 CB THR 308 2701 3586 3626 242 -361 -456 2156 OG1 THR ATOM 308 12.140 0.751 56.028 1.000 32.90 ANISOU 2156 OG1 THR 308 4146 4188 4167 504 745 ATOM 2157 CG2 THR 308 13.577 1.594 54.256 1.000 31.43 ANISOU 2157 CG2 THR 308 3193 4047 4702 -577 -132 -538 ATOM 2158 N SER 309 10.850 -1.591 53.217 1.000 24.73 ANISOU 2158 N SER 309 2934 2092 4370 94 -574 -391 2159 CA SER 309 10.199 -2.897 53.230 1.000 25.19 ANISOU 2159 CA SER 309 3793 2464 3316 -485 451 -230 ATOM 2160 C SER 309 10.466 -3.691 54.512 1.000 24.06 ANISOU 2160 C SER 309 2360 2888 3893 302 107 3 5 MOTA 2161 0 SER 309 11.565 -3.621 55.084 1.000 34.54 ANISOU 2161 O SER 309 3626 2131 7366 -76 -1944 - 3 4 MOTA 2162 CB SER 309 10.639 -3.700 52.012 1.000 26.52 ANISOU 2162 CB SER 309 3970 2159 580 - 366 3948 167 ATOM 2163 OG SER 309 10.217 -5.039 52.148 1.000 26.34 ANISOU 2163 OG SER 309 3198 2207 -844 - 2604604 156 MOTA 2164 N LYS 310 9.494 -4.458 54,961 1,000 24,99 ANISOU 2164 N LYS 310 3172 2459 3864 160 262 366 ATOM 2165 CA LYS 310 9.651 -5.339 56.125 1.000 28.38 ANISOU 2165 CA LYS 310 4191 3167 3427 764 278 281 MOTA 2166 C

-6.768 55.711 1.000 26.07

310 9.941

LYS

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- 84 -
ANISOU 2166 C
                   LYS
                         310 3371
                                       2687
                                                 3846
                                                         168
                                                                -290 5 7 7
ATOM
         2167 0
                   LYS
                         310 10.150
                                      -7.684 56.515 1.000 33.48
ANISOU 2167 O
                   LYS
                         310 5267
                                       3056
                                                 4400
                                                         -66
                                                                -450 1073
ATOM
         2168 CB
                   LYS
                         310 8.299
                                       -5.367
                                                56.858 1.000 37.77
ANISOU 2168 CB
                   LYS
                         310 5736
                                       4695
                                                         299
                                                3921
                                                                1818 1 8
MOTA
         2169 CG
                   LYS
                         310 8.014
                                     -4.214
                                               57.806 1.000 40.55
ANISOU 2169 CG
                   LYS
                         310 6395
                                      4716
                                                4295
                                                         1525
                                                                1524 1 0 1
ATOM
         2170 CD
                   LYS
                         310 6.798
                                       -4.537
                                                58.649 1.000 44.24
ANISOU 2170 CD
                   LYS
                         310 9091
                                      4224
                                                3495
                                                         1053
                                                                2816 5 8 4
ATOM
         2171 CE
                   LYS
                         310 6.722
                                       -6.109 58.818 1.000 59.12
ANISOU 2171 CE
                   LYS
                         310 9281
                                      4577
                                                8606
                                                         766
                                                                -82 2478
ATOM
        2172 NZ
                   LYS
                         310 6.088
                                      -6.563
                                                60.089 1.000 55.80
ANISOU 2172 NZ
                   LYS
                         310 4884
                                                10577
                                      5742
                                                         287
                                                                -947 4796
ATOM
         2173 N
                         311 9.896
311 2190
                   ALA
                                       -7.030 54.410 1.000 22.45
ANISOU 2173 N
                   ALA
                                       2402
                                                3939
                                                         10 52 2 6 9

    311
    2190
    2402
    3939
    10 52 2 6 9

    311
    10.360
    -8.369
    53.972
    1.000
    31.89

    311
    3771
    2594
    5753
    434
    -516 - 4

    311
    11.909
    -8.459
    53.833
    1.000
    23.30

    311
    3907
    2328
    2616
    1393
    -593
    1

    311
    9.619
    -8.665
    52.674
    1.000
    27.94

    311
    2407
    2878
    5329
    -355
    542
    -6

ATOM
        2174 CA
                  ALA
ANISOU 2174 CA
                  ALA
                                                               -516 - 421
        2175 C
ATOM
                   ALA
ANISOU 2175 C
                   ALA
                                                               -593 1 1 2
ATOM
        2176 CB
                  ALA
ANISOU 2176 CB
                  ALA
                        501 -6.477
502 -9.349
503 -1
                                               5329 -355
                                                               542 - 672
MOTA
        2177 OW
                                      10.237 44.256 1.000 15.66
16.189 51.010 1.000 19.26
                  HOH
ATOM
        2178 OW
                  HOH
                         503 -1.489 3.653
ATOM
        2179 OW
                  HOH
                                               34.560 1.000 15.78
50.182 1.000 16.19
MOTA
        2180 OW
                  HOH
                         504 -10.499 18.731
ATOM
        2181 OW
                  HOH
                         505 -8.612 16.958
                                               47.640 1.000 17.30
42.881 1.000 19.05
MOTA
        2182 OW
                         506 -10.255 20.839
                  HOH
ATOM
                        507 2.096
        2183 OW
                  HOH
                                       1.076
                                                32.810 1.000 29.32
ATOM
        2184 OW
                  HOH
                        508 -0.284 4.743
                                                41.885 1.000 13.93
        2185 OW
                        509 -8.525 18.553 42.416 1.000 21.33
ATOM
                  HOH
ATOM
        2186 OW
                  НОН
                        510 3.165
                                      2.604
                                                43.488 1.000 24.59
ATOM
        2187 OW
                  HOH
                         511 -6.282 19.386
                                               52.341 1.000 18.98
ATOM
        2188 OW
                  HOH
                        512 -6.826 24.638
                                               46.833 1.000 21.77
ATOM
        2189 OW
                  HOH
                         513 10.510 -4.344
                                               46.092 1.000 25.88
ATOM
        2190 OW
                  HOH
                         514 -0.806 16.964
                                               40.372 1.000 16.54
        2191 OW
ATOM
                         515 -1.269 18.855
                  HOH
                                               42.411 1.000 15.76
ATOM
        2192 OW
                  HOH
                         516 14.277
                                      -5.146 40.175 1.000 15.53
ATOM
        2193 OW
                         517 -0.123 21.538 40.640 1.000 17.22
                  HOH
ATOM
        2194 OW
                  HOH
                         518 13.131
                                      -0.967 51.791 1.000 31.17
ATOM
        2195 OW
                  HOH
                         519 11.009 2.875
                                                45.599 1.000 20.20
                        520 5.789
521 2.168
ATOM
        2196 OW
                  HOH
                                      13.543
                                               45.996 1.000 17.36
ATOM
        2197 OW
                  НОН
                                      19.767
                                               55.925 1.000 20.41
ATOM
        2198 OW
                  нон
                        522 8.487
                                      15.960 34.949 1.000 15.40
ATOM
        2199 OW
                  НОН
                        523 10.794
                                                29.921 1.000 19.99
                                      12.697
ATOM
        2200 OW
                  HOH
                        524 -11.722 19.112
                                               44.516 1.000 19.82
ATOM
        2201 OW
                  HOH
                        525 1.672
                                      -2.081
                                                35.124 1.000 16.29
ATOM
        2202 OW
                        526 9.651
                  HOH
                                       15.283
                                                32.342 1.000 20.37
ATOM
        2203 OW
                  HOH
                         527 28.749
                                       31.187
                                                52.019 1.000 18.53
ATOM
        2204 OW
                  HOH
                        528 15.326
                                       11.252
                                                32.041 1.000 19.60
        2205 OW
MOTA
                  HOH
                        529 26.897
                                       26.984
                                                52.035 1.000 19.86
ATOM
        2206 OW
                  HOH
                        530 13.528
                                      11.592
                                                50.915 1.000 16.17
ATOM
        2207 OW
                        531 25.631
                  HOH
                                      32.409
                                                52.682 1.000 19.20
MOTA
        2208 OW
                  HOH
                        532 18.287
                                                52.185 1.000 18.49
39.395 1.000 18.09
                                       6.835
ATOM
        2209 OW
                  HOH
                        533 12.635
                                      29.035
ATOM
        2210 OW
                  HOH
                        534 10.797
                                       31.968
                                                45.659 1.000 20.66
ATOM
        2211 OW
                  HOH
                        535 10.167
                                       24.890
                                                33.567 1.000 19.12
ATOM
        2212 OW
                  нон
                        536 23.530
                                      24.122
                                                58.531 1.000 20.39
ATOM
        2213 OW
                  HOH
                        537 23.358
                                       12.639
                                                35.292 1.000 22.61
MOTA
        2214 OW
                  нон
                        538 25.879
                                      28.699
                                                50.264 1.000 19.44
MOTA
        2215 OW
                  нон
                        539 11.674
                                      16.559
                                                30.502 1.000 18.57
ATOM
        2216 OW
                  HOH
                        540 18.515
                                      27.775 40.042 1.000 22.23
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MOTA 2217 OW нон 541 21.233 20.367 33.996 1.000 21.45 MOTA 2218 OW HOH 542 22.826 32.643 53.094 1.000 19.38 ATOM 2219 OW нон 543 19.670 22.387 35.310 1.000 20.05 ATOM 2220 OW нон 544 -13.591 21.996 61.494 1.000 49.93 MOTA 2221 OW нон 545 21.295 11.783 55.080 1.000 20.04 ATOM 2222 OW нон 546 5.431 2.533 51.677 1.000 28.11 547 17.311 ATOM 2223 OW HOH 25.489 32.148 1.000 24.38 ATOM 2224 OW HOH 548 17.427 7.744 33.008 1.000 20.78 ATOM 2225 OW нон 549 11.656 23.874 58.194 1.000 23.39 ATOM 2226 OW HOH 550 8.037 14.987 53.326 1.000 33.52 ATOM 2227 OW НОН 551 1.354 14.574 33.889 1.000 21.05 2228 OW 552 11.203 20.116 ATOM НОН 63.686 1.000 24.59 2229 OW 553 2.671 ATOM нон 21.240 34.245 1.000 34.51 ATOM 2230 OW HOH 554 6.339 30.751 1.000 26.36 19.832 2231 OW ATOM HOH 555 26.611 24.519 55.570 1.000 21.22 2232 OW ATOM НОН 556 27.669 17.156 53.039 1.000 25.86 ATOM 2233 OW HOH 557 -14.392 19.977 44.154 1.000 25.03 ATOM 2234 OW HOH 558 14.828 32.652 51.443 1.000 25.23 MOTA 2235 OW НОН 559 17.937 7.207 54.915 1.000 20.59 ATOM 2236 OW 560 10.729 HOH -8.875 31.499 1.000 24.65 ATOM 2237 OW нон 42.613 1.000 22.74 44.166 1.000 27.75 53.556 1.000 25.28 49.697 1.000 23.33 561 6.455 2.298 ATOM 2238 OW нон 562 13.784 31.245 ATOM 2239 OW HOH 563 17.292 33.470 нон ATOM 2240 OW 564 11.210 1.109 ATOM 2241 OW НОН 565 -11.339 25.246 41.370 1.000 26.08 ATOM 2242 OW HOH -8.375 566 20.363 38.242 1.000 30.07 ATOM 2243 OW HOH 567 3.890 24.604 35.837 1.000 25.86 ATOM 2244 OW HOH 568 5.334 11.875 43.937 1.000 25.45 ATOM 2245 OW HOH 569 7.861 22.385 64.046 1.000 28.98 ATOM 2246 OW HOH 570 7.754 -1.508 30.848 1.000 24.72 ATOM 2247 OW HOH 28.471 1.000 33.06 571 6.297 3.583 ATOM 2248 OW HOH 572 -15.790 28.800 51.855 1.000 30.09 MOTA 2249 OW нон 573 -5.388 20.310 38.883 1.000 23.64 MOTA 2250 OW HOH 574 17.657 21.059 29.053 1.000 24.31 MOTA 2251 OW нон 575 8.763 20.920 66.102 1.000 24.81 ATOM 2252 OW НОН 576 10.135 27.617 58.357 1.000 25.12 ATOM 2253 OW HOH 577 7.795 1.060 29.730 1.000 29.00 ATOM 2254 OW НОН 578 22.601 19.580 61.946 1.000 28.66 ATOM 579 8.859 2255 OW нон 4.744 27.898 1.000 26.12 580 4.937 MOTA 2256 OW HOH 3.932 48.882 1.000 26.29 ATOM 2257 OW HOH 581 17.096 5.891 35.057 1.000 23.31 582 -16.337 31.047 583 7.652 24.826 584 7.174 24.915 585 23.452 10.614 MOTA 2258 OW HOH 64.719 1.000 54.01 ATOM2259 OW нон 52.106 1.000 27.23 ATOM 2260 OW нон 29.292 1.000 26.60 ATOM 2261 OW нон 55.439 1.000 26.42 586 12.640 587 6.204 MOTA 2262 OW HOH 26.413 58.676 1.000 27.15 ATOM 2263 OW HOH 21.166 62.094 1.000 24.65 ATOM 2264 OW 588 2.385 37.616 1.000 19.92 45.738 1.000 38.29 45.065 1.000 30.46 HOH 0.810 ATOM 2265 OW HOH 589 32.930 28.236 590 -12.045 28.716 589 32.930 ATOM 2266 OW HOH ATOM 2267 OW 36.120 1.000 27.12 43.344 1.000 26.67 HOH 591 0.219 13.612 ATOM 2268 OW нон 592 -2.525 3.881 48.055 1.000 19.59 42.057 1.000 25.53 46.425 1.000 22.12 ATOM 2269 OW нон 593 7.533 13.297 28.355 ATOM 2270 OW нон 594 -1.575 MOTA 2271 OW 595 11.209 HOH -1.188 ATOM 2272 OW HOH 596 5..684 28.451 1.000 27.97 -7.000 ATOM 597 28.868 2273 OW HOH 19.406 51.825 1.000 27.72 ATOM 2274 OW 598 13.432 57.904 1.000 31.12 HOH 2.493 MOTA 2275 OW HOH 599 8.196 7.483 27.148 1.000 29.99 MOTA 2276 OW нон 600 20.809 63.369 1.000 36.86 19.088 MOTA 2277 OW нон 601 21.352 34.614 1.000 30.60 10.656

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- 86 -ATOM 2278 OW HOH 602 2.891 7.196 30.899 1.000 25.41 ATOM 2279 OW HOH 603 8.260 26.496 34.561 1.000 35.71 ATOM 2280 OW HOH 604 22.300 13.959 31.378 1.000 32.53 ATOM 2281 OW HOH 605 15.689 35.750 48.870 1.000 31.17 ATOM 2282 OW HOH 606 7.219 15.638 30.914 1.000 27.80 ATOM 2283 OW 607 -3.237 HOH 14.604 47.092 1.000 20.96 ATOM 2284 OW 608 17.543 HOH 10.581 33.561 1.000 23.51 ATOM 2285 OW HOH 609 -1.899 36.370 44.261 1.000 32.64 ATOM 2286 OW HOH 610 26.095 14.431 43.803 1.000 19.19 ATOM 2287 OW нон 611 27.664 13.183 41.954 1.000 26.48 2288 OW MOTA HOH 612 4.302 34.604 49.981 1.000 24.70 MOTA 2289 OW HOH 613 -15.580 27.012 46.728 1.000 42.45 ATOM 2290 OW HOH 614 1.615 35.544 50.347 1.000 23.78 MOTA 2291 OW HOH 615 -10.137 34.259 49.033 1.000 23.94 ATOM 2292 OW HOH 616 26.084 6.502 57.657 1.000 39.32 АТОМ 2293 OW HOH 617 -15.962 20.656 46.340 1.000 25.94 MO1.A 2294 OW HOH 618 6.113 29.517 40.143 1.000 29.43 MOTA 2295 OW HOH 619 19.797 4.627 51.313 1.000 27.15 2296 OW ATOM HOH 620 -1.748 11.315 48.716 1.000 21.83 ATOM 2297 OW 621 11.099 622 28.352 HOH 34.289 44.259 1.000 27.15 ATOM 2298 OW HOH 14.351 37.877 1.000 41.48 2299 OW ATOM HOH 623 -2.826 36.968 57.149 1.000 32.75 624 16.983 625 16.780 626 1.632 ATOM 2300 OW HOH 9.258 29.962 1.000 32.82 ATOM 2301 OW HOH 29.213 38.384 1.000 27.96 ATOM 2302 OW HOH 17.213 33.689 1.000 23.17 ATOM 2303 OW 627 33.536 HOH 23.640 45.028 1.000 41.91 ATOM 2304 OW нон 628 23.821 6.059 50.174 1.000 34.22 2305 OW MOTA 629 3.482 HOH 2.785 46.751 1.000 39.07 ATOM 2306 OW HOH 630 20.218 24.803 60.918 1.000 50.12 2307 OW ATOM HOH 631 3.366 16.272 30.698 1.000 31.50 ATOM 2308 OW 11.791 25.782 HOH 632 18.871 31.384 1.000 30.78 ATOM 2309 OW HOH 633 4.455 58.823 1.000 32.14 ATOM 2310 OW 40.319 1.000 40.13 43.466 1.000 50.48 60.797 1.000 26.58 HOH 634 24.721 5.202 ATOM 2311 OW HOH 635 19.623 35.238 ATOM 2312 OW нон 636 22.789 26.242 ATOM 2313 OW HOH 637 7.008 -4.80954.039 1.000 ATOM 2314 OW HOH 638 -15.821 18.362 42.559 1.000 29.61 ATOM 2315 OW HOH 639 -11.847 15.711 52.841 1.000 25.21 ATOM 2316 OW НОН 640 -1.948 13.411 35.401 1.000 30.41 ATOM 2317 OW НОН 641 -14.293 21.937 42.145 1.000 27.58 ATOM 2318 OW HOH 642 18.216 20.839 66.863 1.000 31:23 ATOM 2319 OW HOH 643 9.836 36.288 48.178 1.000 44.21 MOTA 2320 OW HOH 644 3.510 16.168 66.253 1.000 33.82 ATOM 2321 OW HOH 645 7.571 33.398 41.687 1.000 37.96 ATOM 2322 OW HOH 646 0.780 21.844 36.729 1.000 31.71 ATOM 2323 OW HOH 647 21.244 -2.321 35.579 1.000 32.40 ATOM 2324 OW HOH 648 3.027 25.244 69.907 1.000 36.84 ATOM 2325 OW нон 649 1.129 25.273 66.516 1.000 35.42 ATOM 2326 OW HOH 650 14.646 7.560 60.327 1.000 46.42 MOTA 2327 OW HOH 651 -8.287 26.381 37.998 1.000 29.17 MOTA 2328 OW HOH 652 10.153 23.548 67.703 1.000 31.50 ATOM 2329 OW нон 653 28.906 22.258 38.969 1.000 32.66 ATOM 2330 OW HOH 654 13.568 -4.482 31.517 1.000 26.94 ATOM 2331 OW 655 -12.635 17.106 55.637 1.000 26.85 656 2.698 5.770 50.702 1.000 29.05 HOH ATOM 2332 OW HOH... 656 2.698 ATOM 2333 OW HOH 657 -1.384 7.487 46.512 1.000 36.52 MOTA 2334 OW 658 3.880 HOH 19.246 31.498 1.000 31.50 ATOM 2335 OW HOH 659 -1.400 31.406 64.001 1.000 56.62 ATOM 2336 OW HOH 660 11.416 23.260 65.229 1.000 32.69 2337 OW ATOM HOH 661 15.994 14.673 25.680 1.000 36.46 2338 OW ATOM HOH 662 28.572 21.242 53.423 1.000 39.06

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2339 OW
                 HOH
ATOM
                      663 19.354
                                  0.465
                                           27.273 1.000 44.56
MOTA
       2340 OW
                 нон
                      664 24.969
                                   27.026
                                           38.838 1.000 35.41
       2341 OW
ATOM
                 нон
                      665 24.294
                                   7.488
                                           55.914 1.000 32.97
ATOM
       2342 OW
                 нон
                      666 19.540
                                  7.882
                                           31.178 1.000 30.04
ATOM
       2343 OW
                 HOH
                      667 -9.236
                                           57.241 1.000 39.20
67.496 1.000 38.83
                                  32.988
       2344 OW
ATOM
                 нон
                      668 2.098
                                  18.351
ATOM
       2345 OW
                 HOH
                      669 11.390
                                           56.270 1.000 37.56
                                  3.245
       2346 OW
ATOM
                HOH
                      670 -21.413 24.449
                                           52.026 1.000 44.66
MOTA
       2347 OW - HOH
                      671 -14.575 19.220
                                           55.240 1.000 30.91
ATOM
       2348 OW
                 HOH
                      672 32.112
                                  25.958
                                           43.051 1.000 33.34
MOTA
       2349 OW
                нон
                      673 -15.050 31.151
                                           53.232 1.000 34.71
MOTA
       2350 OW
                нон
                      674 2.941
                                  -1.607
                                           30.245 1.000 34.63
       2351 OW
MOTA
                HOH
                      675 26.951
                                  14.544
                                           34.757 1.000 49.17
MOTA
       2352 OW
                нон
                      676 14.707
                                  30.669
                                           39.386 1.000 30.55
       2353 OW
MOTA
                HOH
                      677 5.203
                                  18.009
                                           68.080 1.000 43.41
MOTA
       2354 OW
                HOH
                      673 14.151
                                  7.965
                                           26.591 1.000 38.80
       2355 OW
ATOM
                НОН
                      679 24.470
                                  24.261
                                           41.443 1.000
                                                         31.28
       2356 OW
ATOM
                 HOH
                      680 17.540
                                  2.410
                                           28.478 1.000 34.31
ATOM
       2357 OW
                HOH
                      681 25.992
                                  20.593
                                           34.326 1.000 39.66
       2358 OW
ATOM
                HOH
                      682 13.802
                                  35.357
                                           44.421 1.000 34.06
       2359 OW
ATOM
                нон
                      683 1.087
                                           45.456 1.000 35.39
                                  2.355
ATOM
       2360 OW
                нон
                      684 22.443
                                  34.538
                                           42.053 1.000 33.55
ATOM
       2361 OW
                HOH
                      685 4.419
                                  4.720
                                           27.356 1.000 48.02
ATOM
       2362 OW
                 HOH
                      686 -15.830 34.507
                                           51.877 1.000 50.63
                      687 -15.217 29.490
MOTA
       2363 OW
                 HOH
                                           48.887 1.000 33.54
ATOM
       2364 OW
                 НОН
                      688 36.808 21.183
                                           46.206 1.000 44.97
       2365 OW
ATOM
                 НОН
                      689 3.756
                                  1.312
                                           29.272 1.000 35.16
ATOM
       2366 OW
                 нон
                      690 18.802
                                  13.646
                                           27.901 1.000 30.08
       2367 OW
ATOM
                 HOH
                      691 6.997
                                  17.521
                                           29.313 1.000 47.70
                      692 13.725
693 22.369
ATOM
       2368 OW
                HOH
                                  16.327
                                           69.105 1.000 36.97
ATOM
       2369 OW
                HOH
                                  22.161
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ATOM
       2370 OW
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695 19.351
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30.744 1.000 34.21
29.376 1.000 36.59
57.304 1.000 38.35
                HOH
                                  31.620
       2371 OW
ATOM
                HOH
                                  23.082 22.414
ATOM
       2372 OW
                HOH
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       2373 OW
ATOM
                нон
                      697 28.700
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ATOM
       2374 OW
                HOH
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43.200 1.000 43.20
68.342 1.000 39.95
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ATOM
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       2377 OW
ATOM
                нон
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ATOM
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ATOM
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                нон
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MOTA
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MOTA
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                HOH
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                                  26.799
                                           66.321 1.000 43.74
                 HOH
ATOM
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MOTA
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ATOM
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       2398 OW
MOTA
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                                   0.000
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       2399 OW
ATOM
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ATOM	2401	OW	нон	725	19.289	24.195	33.321		32.28
MOTA	2402	OW	HOH	726	0.000	0.000	31.798	0.330	50.38
ATOM	2403	OW	нон	727	-1.223	38.165	59.229	1.000	31.24
ATOM	2404	OW	HOH	728	22.035	38.254	45.742	1.000	48.21
ATOM	2405	OW	HOH	729	28.388	16.248	63.044	1.000	31.59
ATOM	2406	OW	HOH	730	0.000	0.000	45.995	0.330	36.14
ATOM	2407	WO	HOH	731	2.984	29.007	40.091	1.000	36.08
ATOM	2408	OW	HOH	732	5.297	15.835	27.318	1.000	41.53
MOTA	2409	OW	HOH	733	17.347	10.778	27.373	1.000	35.27
ATOM	2410	OM	HOH	734	29.417	14.607	53.127	1.000	40.12
ATOM	2411	OW	HOH	735	4.222	-8.636	27.012	1.000	35.22
ATOM	2412	OW	HOH	736	-9.949	17.712	62.813	1.000	34.43
ATOM	2413	OM	HOH	737	13.960	-10.203	55.259	1.000	31.79
ATOM	2414	OM	HOH	738	11.831	-1.522	49.308	1.000	25.22
ATOM	2415	OW	HOH	739	2.896	4.247	29.596	1.000	38.64
ATOM	2416	OW	HOH	740	10.959	13.759	25.528	1.000	61.86
ATOM	2417	OW	HOH	741	0.864	17.227	30.557	1.000	50.71
ATOM	2418	OW	HOH	742	31.755	18.949	52.065	1.000	40.48
MOTA	2419	OM	HOH	743	21.678	-0.485	28.218	1.000	43.23
MOTA	2420	OW	HOH	744	10.583	16.397	75.211	1.000	45.04
ATOM	2421	OW	HOH	745	7.480	7.996	78.287	1.000	57.64
MOTA	2422	OM	HOH	746	24.067	35.122	40.297	1.000	41.95
ATOM	2423	OW	HOH	747	7.804	10.269	78.332	1.000	49.63
ATOM	2424	OM	HOH	748	22.131	40.645	45.806	1.000	49.69
ATOM	2425	OM	HOH	749	14.850	-4.647	33.872	1.000	42.88
MOTA	2426	OW	HOH	750	-12.930	32.504	55.211	1.000	37.15
ATOM	2427	OW	HOH	751	-4.832	35.986	43.333	1.000	44.39
ATOM	2428	OW	HOH	752	19.834	33.566	56.449	1.000	31.56
MOTA	2429	OM	HOH	753	3.363	22.310	29.844	1.000	42.02
ATOM	2430	OM	HOH	754	25.594	4.030	34.174	1.000	51.90
ATOM	2431	OW	HOH	755	28.036	35.859	46.448	1.000	39.50
ATOM	2432	OW	HOH	756	-12.951	16.294	61.787	1.000	40.94
MOTA	2433	OW	HOH	757	-10.870	26.452	38.737	1.000	44.85
MOTA	2434	OM	HOH	758	13.216	12.896	70.729	1.000	63.42
MOTA	2435	OW	HOH	759	-0.403	21.161	74.990	1.000	38.96
ATOM	2436	OM	HOH	760	-7.025	32.526	64.316	1.000	39.64
ATOM	2437	OW	HOH	761	-15.459	19.739	58.090	1.000	40.84
MOTA	2438	WO	HOH	762	-4.964	36.577	59.068	1.000	48.64
MOTA	2439	OM	HOH	763	26.807	35.717	50.036	1.000	43.54
MOTA	2440	WO	HOH	764	19.542	7.083	65.538	1.000	41.41
ATOM	2441		HOH	765	3.709	35.837	42.709	1.000	33.78
MOTA	2442	OW	HOH	766	0.431	33.688	40.172	1.000	36.91
MOTA	2443	OW.	HOH	767	18.620	5.064	64.617	1.000	45.76
MOTA	2444	OM	НОН	768	35.526	19.792	41.322	1.000	52.54
MOTA	2445	OW	HOH	769	19.671	7.789	67.717	1.000	43.44
ATOM	2446	OW	нон	770	3.562	12.048		1.000	
ATOM	2447	OW	нон	771	20.245	35.637		1.000	52.16
ATOM	2448	OM	НОН	772	-20.588	25.640		1.000	58.60
ATOM	2449	OM	HOH	773	1.556	37.342		1.000	
MOTA	2450	OW	нон	774	8.340	0.668		1.0001	
MOTA	2451	OW	НОН	775	27.160	2.372		1.000	
ATOM	2452	OM	НОН	776	6.575	19.271		1.000	

ATOM	2453	OW	нон	777	-17.605	29.205	62.661	1.000	56.83
ATOM	2454	OW	нон	778	7.616	6.902	24.722	1.000	61.34
MOTA	2455	OW	нон	7 79	19.749	10.700	68.006	1.000	65.22
MOTA	2456	W	НОН	780	7.281	-5.270	50.090	1.000	50.00
MOTA	2457	W	HOH	781	-6.809	28.483	40.515	1.000	50.00
ATOM	2458	W	HOH	782	9.990	17.263	38.636	1.000	50.00
MOTA	2459	W	НОН	783	5.767	-2.331	28.939	1.000	50.00
ATOM	2460	W	нон	784	11.694	-0.118	24.984	1.000	50.00
ATOM	2461	W	нон	785	24.442	7.952	47.994	1.000	50.00
ATOM	2462	W	нон	786	14.251	36.889	46.491	1.000	50.00
ATOM	2463	W	НОН	787	5.759	26.477	33.851	1.000	50.00
ATOM	2464	W	нон	788	-11.816	22.606	40.795	1.000	50.00
ATOM	2465	W	нон	789	-2.531	5.579	45.829	1.000	50.00
ATOM	2466	W	НОН	790	-13.002	32.034	46,612	1.000	50.00
MOTA	2467	W	нон	791	2.230	3.555	48.985	1.000	50.00
ATOM	2468	W	HOH	792	9.397	13.464	28.121	1.000	50.00
ATOM	2469	W	нон	793	28.257	10.442	42.781	1.000	50.00
MOTA	2470	W	НОН	794	4.652	17.944	59.241	1.000	50.00
ATOM	2471	W	HOH	795	5.977	15.287	79.554	1.000	50.00
ATOM	2472	W	HOH	796	30.501	11.852	47.616	1.000	50.00
ATOM	2473	W	НОН	797	5.625	14.258	54.367	i.000	50.00
ATOM	2474	W	НОН	798	23.942	20.228	33.277	1.000	50.00
ATOM	2475	W	нон	799	10.164	14.642	58.997	1.000	50.00
MOTA	2476	W	нон	800	7.807	31.943	52.999	1.000	50.00
ATOM	2477	W	нон	801	23.377	9.361	34.817	1.000	50.00
ATOM	2478	W	нон	802	21.193	9.722	32.004	1.000	50.00
ATOM	2479	W	нон	803	34.928	14.644	46.038	1.000	50.00
ATOM ATOM	2480	W	нон	804		16.684	34.445	1.000	50.00
ATOM	2481	W	нон		7.008	-2.049	51.872	1.000	
ATOM	2482	W	НОН	806	25.363	7.860	45.531	1.000	50.00
ATOM	2483 2484	W	НОН	807	30.704	8.207	55.971	1.000	50.00
ATOM	2485	W W	HOH	808	33.072	24.900	40.599	1.000	50.00
ATOM	2486	W	нон нон		-15.577	19.225	63.152	1.000	50.00
ATOM	2487	W	нон	810 811	6.072 -7.214	18.137	23.603	1.000	50.00
ATOM	2488	W	НОН	812	5.509	39.940	55.639	1.000	50.00
ATOM	2489	W	нон		33.845	18.517 9.908	74.919	1.000	50.00
ATOM	2490	W	нон	814	0.421	35.779	56.672	1.000	50.00
ATOM	2491	W	нон	815	35.282	21.705	42.931	1.000	50.00
ATOM	2492	W	нон	816	39.344	22.173	48.656	1.000	50.00
ATOM	2493	W	нон	817	-5.192	39.820	46.871	1.000	50.00
ATOM	2494	W	нон	818	30.199	13.039	60.056	1.000	50.00
ATOM	2495	W	нон	819	-4.860	36.454	33.383	1.000	50.00
ATOM	2496	W	нон		-14.599	17.407	58.382	1.000	
ATOM	2497	W	нон	821	1.340	-0.111	41.711	1.000	50.00
ATOM	2498	W	нон		34.512	23.218	52.108	1.000	50.00
ATOM	2499	W	нон	823	32.136	12.571	52.108	1.000	
ATOM	2500	W	нон	824	13.525	-6.549	29.838	1.000	50.00
ATOM		W	нон	825	6.072	-4.141	27.534	1.000	50.00
	·						- 1		50.00

STRUCTURE B

ANISOU 24 ATOM 25 ANISOU 25 ATOM 26 ANISOU 26 ATOM 27 ANISOU 27 ATOM 28 ANISOU 28 ATOM 29 ANISOU 29 ATOM 30	MECCOCOSSCCCCCOONNCCOOOCCCOONNCCCOOCCCOONNCCCOOCCCOONNCCCOOCCCOONNCCCOOCCCOONNCCCOOCCCOONNCCCOOCCCOOONNCCCOOCCCOOOCCCOOONNCCCCOOCCCOOOCCCCOOOCCCCOOONNCCCOOCCCCOOOCCCCOOOCCCCOOOCCCCOOOCCCCOOONNCCCCOOCCCCOOOCCCCOOOCCCCOOOCCCCOOOCCCCOOOCCCC	111111111111122222222222222233333333333	31.63.03.06.25.04.25.05.05.05.05.05.05.05.05.05.05.05.05.05	3634 15.176 4393 15.029 2636 14.764 2494 13.762 2209 14.220 2620 12.412 1863 16.061 2548 16.044 2485 17.181 2456 19.650 2429 19.484 2812 20.942 218.577 2760 18.264	59.663 59.663 59.556 5094 58.379 4489 60.597 3807 61.414 4495 62.758 3989 61.315 7630.55 7630.55 7630.39 7597.33 60.32 7597.33 61.55 61.	1113
ATOM 31	O THR	4	2668	2629	2902	246 -560 -659
	N VAL	5	24.104	19.049	59.340	1.000 15.88

- 91 -ANISOU 31 N VAL 5 2505 2021 1508 -613 -630 - 162 ATOM 32 CA VAL 5 23.211 19.385 58.211 1.000 14.80 ANISOU 32 CAVAL 5 2463 1893 -594 -473 - 87 1266 MOTA 33 CB VAL 5 21.742 19.402 58.606 1.000 16.09 ANISOU 33 CB VAL 5 2476 1881 -412 -406 5 0 2 1757 ATOM 34 CG1 VAL 5 20.855 19.846 57.447 1.000 14.91 ANISOU 34 CG1 VAL 5 2458 1859 1337 9 -102 197 ATOM 3.5 CG2 VAL 5 21.310 17.994 59.074 1.000 21.15 CG2 VAL ANISOU 35 5 3015 2345 2677 -700 -418 1198 MOTA 3 ნ С 5 VAL 20.762 57.694 1.000 17.70 23.639 ANISOU 36 С VAL 5 2893 2085 1749 -1137 -713 1 0 3 MOTA 37 0 5 VAL 23.532 21.759 58.419 1.000 17.35 ANISOU 37 0 VAL 5 2566 1978 2050 -698 -650 1 0 5 MOTA 38 И PRO 6 20.845 56.479 1.000 13.23 24.150 ANISOU 38 N PRO 6 1597 1334 2097 -162 -658 4 0 9 CD PRO ATOM 39 6 24.302 19.770 55.484 1.000 15.56 ANISOU 39 CD PRO 6 1887 1850 2176 -309 -383 2 7 7 ATOM 40 CAPRO 6 24.667 22.137 56.005 1.000 14.49 ANISOU 40 CAPRO 6 1332 1740 2432 -218 -536 5 2 2 ATOM 41 21.722 54.847 1.000 18.21 CB PRO 6 25.571 ANISOU 41 CB 2294 1740 2886 -224 130 434 25.132 20.378 54.409 1.000 20.37 PRO б ATOM 42 PRO 6 CGANISOU 42 CG PRO 6 2708 2632 2399 -1078 38 - 61 ATOM 43 C PRO 6 23.576 23.091 55.510 1.000 14.59 ANISOU 43 C PRO 6 1388 1712 2443 -406 -786698 ATOM PRO 44 0 6 22.408 22.743 55.295 1.000 13.06 ANISOU 44 0 PRO 6 1298 1547 2118 -283 -596 1 5 MOTA 45 N THR 7 24.048 24.326 55.313 1.000 14.56 ANISOU 45 N THR 7 1393. 1678 2463 -380 -565 5 8 7 ATOM 46 CA7 THR 23.288 25.428 54.771 1.000 13.28 ANISOU 46 CA7 THR 1463 1584 -469 -734 4 4 0 1998 ATOM 47 CB 7 THR 23.121 26.572 55.799 1.000 14.44 ANISOU 47 C3 THR 7 1927 1652 1905 -348 -1257 3 2 9 MOTA 48 OG1 THR 7 22.454 26.102 56.998 1.000 18.44 ANISOU 48 OG1 THR 7 3136 2013 1858 -333 -829 1 7 6 49 MOTA CG2 THR 7 22.290 27.719 55.261 1.000 14.98 CG2 THR ANISOU 49 7 1390 1788 2513 -213 -727 4 1 2 MOTA 50 С 7 THR 23.973 26.005 53.539 1.000 14.62 ANISOU 50 C THR 7 1144 2200 2212 -355 -693 7 0 4 MOTA 51 0 7 THR 25.192 26.257 53.600 1.000 17.21 ANISOU 51 0 THR 7 1284 2515 2738 -641 -840 9 7 5 MOTA 52 N PHE 8 23.211 26.222 52.472 1.000 12.32 ANISOU 52 N PHE 8 1165 1596 1919 -314 -534 3 7 0 MOTA 53 CAPHE 8 23.692 26.869 51.283 1.000 13.31 ANISOU 53 CA PHE 8 1554 1531 1971 -60 -295 3 4 3 ATOM 54 CB PHE 8 23.724 25.933 50.067 1.000 13.71 ANISOU 54 CBPHE 8 1479 1705 2025 -136 -232 2 3 4 ATOM 55 CG PHE 8 24.635 24.746 50.258 1.000 13.68 ANISOU 55 CG PHE 8 1225 1716 2257 -185 8 155 ATOM 56 CD1 PHE 8 24.147 23.503 50.628 1.000 14.10 1710 2329 -93 231 2 ANISOU 56 CD1 PHE 8 1317 231 221 MOTA 57 CD2 PHE 8 26.006 24.882 50.079 1.000 17.52 ANISOU 57 CD2 PHE 8 1239 2282 3134 -234 -56 917 MOTA 58 CE1 PHE 8 24.984 22.420 50.812 1.000 15.39 ANISOU 58 CE1 PHE 8 1473 1878 2497 -11 242 MOTA 59 CE2 PHE 8 26.840 23.807 50.271 1.000 17.73 ANISOU 59 CE2 PHE 8 1179 2259 3301 -157 -143 4 2 3 60. MOTA CZPHE 8 22.567 50.654 1.000 17.12 26.348 ANISOU 60 CZPHE 8 1310 2437 2757 24 - 382 978 MOTA 61 C PHE 8 22.821 28.073 50.909 1.000 12.76 ANISOU 61 С PHE 8 1401 1513 1935 -164 -145 4 4 2

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                         22.199
                                 34.259
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ANISOU 79
            CB
                ALA
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                                  1877
                                         2529
                                                 -670
                                                       -674 2 5 9
ATOM
       8 0
            С
                ALA
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                         23.786
                                 32.535
                                         44.831 1.000 16.33
ANISOU 80
            C
                ALA
                     11
                         2319
                                  2255
                                         1629
                                                 -754
                                                       -988 4 3 4
ATOM
       81
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                ALA
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                          24.260
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ANISOU 81
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                ALA
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                                  2559
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                                                       -560 6 1 9
ATOM
       82
            Ν
                GLU
                     12
                          24.558
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                                         45.810 1.000 17.28
ANISOU 82
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                GLU
                     12
                          2686
                                  1994
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                                                 -454
                                                       -1087
MOTA
       83
            CA
                GLU
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                         25.931
                                 31.654
                                         45.752 1.000 16.34
ANISOU 83
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                GLU
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                                  1674
                                                 -474 -889 1 0 3 3
                                         1831
ATOM
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            CB
                GLU
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ANISOU 84
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                GLU
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                                         1808
ATOM
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            CG
                GLU
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                         26.633 32.802
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ANISOU 85
            CG
                GLU
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                          2717
                                 2127
                                         2335
                                                 -1216 -1090 788
ATOM
       86
            CD
                         27.115
                GLU
                      12
                                 32.657
                                         49.342 1.000 21.17
ANISOU 86
            CD
                GLU
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                          3300
                                 2547
                                         2198
                                                 -1182 -1053 7 2 4
ATOM
       87
            OE1 GLU
                      12
                          27.538
                                 31.558 49.756 1.000 22.07
ANISOU 87
            OE1 GLU
                      12
                          2722
                                  3014
                                         2650
                                                 -720 -1365 7 9 7
ATOM
       88
            OE2 GLU
                      12
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                                 33.679 50.059 1.000 29.26
ANISOU 88
            OE2 GLU
                      12
                          5764
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ATOM
       89
            C
                GLU
                      12
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                                 30.402 44.882 1.000 17.16
ANISOU 89
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                GLU
                     12
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ATOM
       90
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                GLU
                     12
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                                  30.317
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ANISOU 90
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                GLU
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                          3200
                                  2388
                                         1583
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ATOM
       91
            Ν
                LEU
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ANISOU 91
                LEU
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                          2176
                                  2300
                                         2104
                                                 -659 -386 9 4
ATOM
       92
            CA
                LEU
                     13
                          25.082
                                  28.252 44.189 1.000 14.00
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- 93 -ANISOU 92 CA LEU 13 1734 1873 1713 -140 -170 4 9 8 93 24.003 27.248 44.620 1.000 15.37 MOTA CB LEU 13 ANISOU 93 CB LEU 13 2205 1838 1795 -375 -149 4 6 5 24.154 26.554 45.967 1.000 14.52 94 CG LEU 13 MOTA ANISOU 94 CG LEU 13 1913 1803 1799 -280 -204 4 4 2 MOTA 95 CD1 LEU 13 22.934 25.680 46.193 1.000 15.15 ANISOU 95 CD1 LEU 13 2174 1817 1766 -433 185 175 25.411 25.690 46.067 1.000 17.54 MOTA 96 CD2 LEU 13 ANISOU 96 CD2 LEU 13 2119 2043 2502 -38 -419 2 7 0 MOTA 97 LEU 13 24.876 28.626 42.725 1.000 16.54 С ANISOU 97 LEU 13 С 2510 2062 1710 -222 -93 565 ATOM 98 O LEU 13 ANISOU 98 O LEU 13 N GLN 14 99 MOTA 99 N GLN 14
100 CA GLN 14
100 CA GLN 14
101 CB GLN 14
101 CB GLN 14
102 CG GLN 14
102 CG GLN 14
103 CD GLN 14
103 CD GLN 14
104 OE1 GLN 14
104 OE1 GLN 14
105 NE2 GLN 14 23.945 29.534 42.472 1.000 16.86 ANISOU 99 1970 2337 2100 -557 -683 8 3 8 MOTA 23.657 30.015 41.132 1.000 18.63 ANISOU 100 2761 2404 1915 -610 -802 5 6 8 MOTA 22.421 30.923 41.130 1.000 19.39 ANISOU 101 3166 2176 2025 -392 -918 9 7 7 MOTA 21.108 30.250 41.460 1.000 19.00 ANISOU 102 2879 2383 1957 -209 -725 4 6 0 19.974 31.227 41.766 1.000 18.83 MOTA ANISOU 103 3139 2118 1897 -6 -1229 4 9 4 ATOM 20.177 32.317 42.314 1.000 26.10 ANISOU 104 3928 2407 3532 -98 -1172 18.745 30.823 41.411 1.000 20.94 -1172 -241 NE2 GLN 14 ATOM 105 ANISOU 105 NE2 GLN 14 2900 2716 2340 -149 -840 4 5 4 106 C 14. ATOM GLN 24.804 30.812 40.525 1.000 20.40 ANISOU 106 C GLN 14 3226 2065 2458 -795 -712 9 3 7 GLN 14 ATOM 107 0 24.812 30.951 39.311 1.000 30.48 GLN 14 ANISOU 107 O 5089 4340 2152 -2337 -898 1 2 1 1 15 ATOM 108 N GLN 25.734 31.309 41.329 1.000 20.35 ANISOU 108 N GLN 15 3252 2452 2030 -1067 -240 4 9 7 ATOM 109 CA GLN 15 32.041 40.884 1.000 21.88 26.909 ANISOU 109 CA GLN 15 3184 3230 1901 -1152 -299 7 8 8 ATOM 110 CB GLN 15 27.288 33.100 41.920 1.000 22.20 ANISOU 110 CB GLN 15 2720 3162 2551 -1131 -770 6 9 1 111 CG ATOM GLN 15 26.450 34.358 41.954 1.000 25.73 ANISOU 111 CG GLN 15 4496 2735 2545 -821 -233 1 2 6 9 ATOM 112 CDGLN 15 26.325 35.021 43.306 1.000 35.76 ANISOU 112 CD GLN 15 6010 3945 3631 -643 -229 -135MOTA 113 OE1 GLN 15 27.145 34.884 44.225 1.000 49.13 ANISOU 113 OE1 GLN 15 8425 5866 4378 -2857 -2197 -564 NE2 GLN 15 ATOM 114 25.255 35.812 43.489 1.000 51.85 NE2 GLN 15 NE2 GLN 15 C GLN 15 C GLN 15 O GLN 15 O GLN 15 N GLY 16 ANISOU 114 7190 5567 6945 62 3066 107 ATOM 115 28.069 31.079 40.625 1.000 23.93 ANISOU 115 -990 145 884 3451 3513 2127 ATOM 29.177 31.448 40.213 1.000 28.95 116 ANISOU 116 3535 4619 2845 -899 510 1225 ATOM 117 16 16 16 16 16 16 N GLY 27.828 29.794 40.891 1.000 25.86 ANISOU 117 N GLY 4089 3282 2457 -889 -36 469 118 ATOM CAGLY 28.812 28.763 40.649 1.000 29.00 ANISOU 118 CAGLY 4785 3562 2671 -677 765 255 ATOM 119 С GLY 29.741 28.546 41.814 1.000 25.45 ANISOU 119 С GLY 3427 3490 -264 1422 6 7 3 2754 ATOM 120 0 GLY 30.805 27.955 41.625 1.000 29.63 ANISOU 120 0 GLY 3925 3267 4068 -66 1997 5 2 3 ATOM N 121 LEU 17 29.387 28.979 43.015 1.000 22.50 ANISOU 121 N LEU 17 3266 2713 -39 2569 923 733 122 CALEU 17 30.234 28.727 44.172 1.000 21.73 ANISOU 122 CALEU 17 2299 2931 3025 -282 867 748

				- 34 -		_
ATOM 123	CB LEU	17	30.124	29.921	45.132	1.000 21.23
ANISOU 123	CB LEU	17	2137			
ATOM 124	CG LEU			2858	3071	-620 669 711
	·	17	30.354	31.274	44.431	1.000 26.12
ANISOU 124	CG LEU	17	2708	2965	4253	-889 1342 9 3 1
ATOM 125	CD1 LEU	17	29.962	32.444	45.305	1.000 29.81
ANISOU 125	CD1 LEU	17	2515	2924	5885	
ATOM 126	CD2 LEU	17	_			-396 464 303
ANISOU 126			31.808	31.350	43.974	1.000 32.84
	CD2 LEU	17	2845	3703	5930	-281 1871 2114
ATOM 127	C LEU	17	29.886	27.456	44.936	1.000 19.36
ANISOU 127	C LEU	17	2081	2819	2455	
ATOM 128	O LEU	17	28.773	26.920		-239 545 580
ANISOU 128	O LEU.		2284	20.920	44.848	1.000 21.11
ATOM 129				3004	2734	-444 107 1055
	N HIS	18	30.838	26.952	45.706	1.000 21.02
ANISOU 129	N HIS	18	2124	2752	3109	-314 193 491
ATOM 130	CA HIS	18	30.678	25.814	46.615	1.000 18.11
ANISOU 130	CA HIS	18	1569	2996	2315	
ATOM 131	CB HIS	18	29.655			-460 -28 361
ANISOU 131	CB HIS			26.149	47.702	1.000 21.25
		18	1731	3332	3010	-45 282 354
	CG HIS	18	29.796	27.515	48.283	1.000 23.28
ANISOU 132	CG HIS	18	2234	3612	2999	211 -46 -20
ATOM 133	CD2 HIS	18	28.898	28.535	48.344	1.000 24.53
ANISOU 133	CD2 HIS	18	3112	3479	2728	
ATOM 134	ND1 HIS	18	30.940	27.977		
ANISOU 134	ND1 HIS				48.895	1.000 26.72
ATOM 135	CE1 HIS	18	2938	4039	3173	-151 -569 3 8
		18	30.756	29.218	49.307	1.000 29.80
ANISOU 135	CE1 HIS	18	4476	3775	3071	-542 -562 2 3 7
ATOM 136	NE2 HIS	18	29.524	29.581	48.985	1.000 30.03
ANISOU 136	NE2 HIS	18	4752	3282	3377	216 -148 3 3 8
ATOM 137	C HIS	18	30.266	24.528	45.917	1.000 18.57
ANISOU 137	C HIS	18	1943	3084	2028	
ATOM 138	O HIS	18	29.594			-951 30 5 9 0
ANISOU 138	O HIS			23.682	46.532	1.000 19.92
ATOM 139		18	1949	3125	2493	-777 -87 995
	N GLN	19	30.647	24.340	44.658	1.000 19.24
ANISOU 139	N GLN	19	2329	2700	2282	-256 298 494
ATOM 140	CA GLN	19	30.119	23.206	43.908	1.000 21.51
ANISOU 140	CA GLN	19	3249	2431	2492	-228 597 3 1 8
ATOM 141	CB GLN	19	30.446	23.307	42.406	1.000 22.89
ANISOU 141	CB GLN	19	3231	3058		
ATOM 142	CG GLN	19			2408	-148 463 244
ANISOU 142			29.738	24.453	41.698	1.000 25.83
	CG GLN	19	3445	3712	2658	-384 -407 5 6 8
ATOM 143	CD GLN	19	28.223	24.470	41.747	1.000 31.56
ANISOU 143	CD GLN	19	3439	4722	3832	-252 -988 3 5 7
ATOM 144	OE1 GLN	19	27.521	23.640	41.153	1.000 38.51
ANISOU 144	OE1 GLN	19	3869	3649	7115	377 -3045 686
ATOM 145	NE2 GLN	19	27.621	25.433		
ANISOU 145	NE2 GLN	19	3303	5695	42.475	1.000 33.32
ATOM 146	C GLN				3663	647 -1109 4 4 9
ANISOU 146		19	30.578	21.873	44.485	1.000 20.32
	C GLN	19	2224	2710	2785	-60 514 394
ATOM 147	0 GLN	19	29.806	20.900	44.473	1.000 19.08
ANISOU 147	0 GLN	19	1888	2451	2910	221 257 743
ATOM 148	N ASP	20		21.761	44.999	1.000 24.09
ANISOU 148	N ASP	20	3001	3507	2645	-773 -507 4 1 5
ATOM 149	CA ASP	2.0				-//3 -50/415
ANISOU 149	CA ASP		32.268	20.498	45.553	1.000 21.82
ATOM 150		20	1707	3811	2774	-327 -58 357
	CB ASP	20	33.780	20.527	45.779	1.000 26.34
ANISOU 150	CB ASP	20	1594	4552	3863	-962 236 490
ATOM 151	CG ASP	20	34.596	20.517	44.503	1.000 34.45
ANISOU 151	CG ASP	20	2531	5859	4701	-1208 1213 - 280
ATOM 152	OD1 ASP	20	34.177	19.982	43.457	1.000 33.11
ANISOU 152	OD1 ASP	20	3768			
ATOM 153	OD2 ASP			4173	4640	-311 1233 - 375
1 55	JUL ASE	20	35.725	21.056	44.532	1.000 49.71

- 95 -ANISOU 153 OD2 ASP 20 3445 9922 5519 -3116 1710 5 3 ATOM 154 C ASP 31.538 20.179 46.862 1.000 21.03 20 ANISOU 154 C ASP 20 1876 2702 3412 -231 616 388 MOTA 155 0 ASP 20 31.118 19.038 47.075 1.000 20.80 ANISOU 155 0 ASP 20 1162 2583 4157 -72 -139 5 5 0 ATOM 156 M GLU 21 31.359 21.177 47.729 1.000 17.88 ANISOU 156 N GLU 21 1218 2751 2824 -263 -148 5 1 1 MOTA 157 C.A. 21 GLU 30.599 20.999 48.965 1.000 16.80 ANISOU 157 CA. GLU 21 1128 2173 3083 -96 46 3 9 4 MOTA 158 CB GLU 21 22.304 49.781 1.000 20.23 30.654 ANISOU 158 CB GLU 21 1366 2620 3701 5 -262 -210 ATOM 159 CG GLU 21 22.669 50.307 1.000 24.60 32.040 ANISOU 159 CG 21 GLU 1660 3325 4359 -221 -654 - 301 MOTA 160 CDGLU 21 23.565 49.402 1.000 28.46 32.860 ANISOU 160 CDGLU 21 1191 4348 5275 -498 -1597 1125 MOTA 161 OE1 GLU 21 33.751 24.294 49.919 1.000 31.17 ANISOU 161 OE1 GLU 21 2360 4428 5057 -1033 -1094 3 4 9 MOTA 162 OE2 GLU 21 32.664 23.590 48.171 1.000 31.16 ANISOU 162 OE2 GLU 21 2734 3901 5203 -1519 -1565 1123 163 20.594 48.689 1.000 16.44 MOTA С GLU 21 29.159 ANISOU 163 С GLU 21 1271 2295 2679 -165 -53 430 MOTA 164 0 19.700 49.329 1.000 14.30 GLU 21 28.599 ANISOU 164 0 GLU 21 1271 2257 -417 -301 3 6 1907 21.257 47.708 1.000 16.14 MOTA 165 Ν . PHE 22 28.548 ANISOU 165 Ν PHE 22 1440 2441 2253 -316 -28 328 ATOM 166 CAPHE 20.947 47.327 1.000 15.36 22 27.155 ANISOU 166 CAPHE 22 1530 2012 .2294 -262 -173 2 8 1 ATOM 167 PHE 26.612 CB 22 21.967 46.343 1.000 15.43 ANISOU 167 CB PHE 22 1863 2056 1944 -316 -247 1 8 4 ATOM 168 CG PHE 22 25.119 21.932 46.077 1.000 15.59 ANISOU 168 CG PHE 22 1822 2141 1962 -299 -170 5 6 1 CD1 PHE ATOM 169 22 24.218 21.987 47.129 1.000 17.03 ANISOU 169 CD1 PHE 22 1923 . 2605 1943 -410 -162 - 40 ATOM 170 CD2 PHE 22 24.606 21.856 44.797 1.000 14.84 ANISOU 170 CD2 PHE 22 1541 2083 2013 51 -94 - 155 CE1 PHE MOTA 171 22 22.861 21.938 46.906 1.000 15.96 ANISOU 171 CE1 PHE 22 1844 1805 2414 -159 -64 176 MOTA 172 CE2 PHE 22 23.243 21.797 44.551 1.000 15.81 ANISOU 172 CE2 PHE 22 1600 1993 2416 -261 -190 -176 ATOM 173 CZPHE 22 22.360 21.853 45.612 1.000 14.18 ANISOU 173 CZPHE 22 1427 1430 2531 -105 -164 3 2 5 ATOM 174 С PHE 22 27.049 19.515 46.792 1.000 16.23 ANISOU 174 C PHE 22 1325 2042 2797 -110 164 102 MOTA 175 0 PHE 22 26.183 18.751 47.229 1.000 13.24 ANISOU 175 0 PHE 22 1411 1743 1876 105 -194 3 9 1 ATOM 176 N ARG 23 27.888 19.097 45.853 1.000 15.45 ANISOU 176 N ARG 23 1585 2313 1971 -167 -80 289 27.865 17.746 45.325 1.000 15.49 MOTA 177 CAARG 23 ANISOU 177 CAARG 809 2443 23 2634 50 -41 ATOM 178 CB ARG 23 28.928 17.539 44.248 1.000 17.81 ANISOU 178 CB ARG 23 . 966 3142 2658 -128 43 -167 MOTA 179 CG ARG 23 28.470 17.928 42.860 1.000 25.86 ANISOU 179 CG ARG 23 2719 4636 2470 -758 -176 - 49 MOTA 180 CD ARG 23 29.485 17.370 41.867 1.000 34.68 ANISOU 180 CDARG 23 5148 4847 3183 -1532 1634 - 548 ATOM 181 ΝE ARG 23 30.660 18.253 41.877 1.000 31.13 ANISOU 181 NΞ ARG 23 2799 4194 4836 305 747 6 6 MOTA 182 CZARG 23 30.703 19.424 41.244 1.000 34.24 ANISOU 182 CZARG 23 2749 4844 5418 -757 239 764 MOTA 183 NH1 ARG 23 29.647 19.856 40.551 1.000 28.06 ANISOU 183 NH1 ARG 23 2714 3685 4263 -721 555 181

						- 96 -		
ATOM	184	NH2	ARG	23	31.830	20.114	41.340	1.000 36.08
ANISOU	184		ARG	23	2261	5328	6121	-562 776 -86
ATOM	185	C	ARG	23	28.045	16.713	46.420	1.000 15.06
ANISOU	185	C	ARG	23	1071	2061	2589	167 -32 -234
ATOM ANISOU		0	ARG ARG	23 23	27.335 1443	15.687	46.410	1.000 16.28
ATOM	187	N	ARG	24	28.952	2244 16.988	2497 47.353	-118 -71 -277 1.000 15.27
ANISOU		N	ARG	24	1024	2156	2623	-52 -21 2 9
ATOM	188	CA	ARG	24	29.193	16.003	48.430	1.000 17.70
ANISOU		CA	ARG	24	1443	2589	2693	275 -2 2 1 5
ATOM	189	CB	ARG	24	30.466	16.422	49.148	1.000 21.11
ANISOU		CB	ARG	24	1244	3486	3289	484 -257 3 8 4
ATOM ANISOU	190	CG CG	ARG	24	31.787	16.217	48.429	1.000 30.46
ANISOU	191	CD	ARG ARG	24 24	1438 32.979	5078 16.537	5057	426 441 308
ANISOU		CD	ARG	24	1163	5831	49.330 5736	1.000 33.50 208 370 458
ATOM	192	NE	ARG	24	33.636	17.804	49.071	1.000 51 . 46
ANISOU		ΝE	ARG	24	5800	7316	6437	-2596 -1688 1165
ATOM	193	CZ	ARG	24	33.973	18.776	49.903	1.000 46.72
ANISOU		CZ	ARG	24	4738	6888	6124	-1719 -1822 1316
ATOM ANISOU	194	NH1	ARG ARG	24 24	33.731	18.728	51.213	1.000 44.24
ATOM	195		ARG	24	2650 34.579	6998 19.871	7160 49.448	-392 1001 8 4 1.000 42.82
ANISOU		NH2		24	5339	4428	6503	513 -991 1 2 1 6
ATOM	196	С	ARG	$\frac{1}{24}$	27.972	15.887	49.334	1.000 17.16
ANISOU		С	ARG	24	1549	2071	2900	129 140 295
ATOM	197	0	ARG	24	27.536	14.779	49.713	1.000 15.38
ANISOU		0	ARG		1706	1890	2247	72 - 388 104
ATOM ANISOU	198	N N	CYS CYS	25 25	27.355	17.011	49.696	
ATOM	199	CA	CYS	25	907 182 26.105	4 21 17.040		54 -386 151 1.00012.45
ANISOU		CA	CYS	25	942 183			
ATOM	200	CB	CYS	25	25.660	18.491	50.697	1.000 11.67
ANISOU		CB	CYS	25	1150	1759	1527	-136 -604 1 8 4
ATOM	201	SG	CYS	25	23.973	18.580	51.425	1.000 14.90
ANISOU		SG	CYS	25	1465	1593	2602	-164 -26 -18
ATOM ANISOU	202	C	CYS CYS	25 25	25.001	16.225		1.000 11.67
ATOM	203	0	CYS	25	893 189 24.360	15.377	45 -2 50.390	83 - 64 - 8 6 1.000 12.73
ANISOU		ŏ	CYS	25	1347	1426	2064	-233 -196 1 2 3
ATOM	204	N	LEU	26	24.798	16.461	48.470	1.000 11.70
ANISOU		N	LEU	26	1102	1530	1814	-128 -390 1
ATOM		CA	LEU	26	23.766	15.716	47.735	1.000 11.11
ANISOU ATOM	205	CA CB	LEU	26	1190	1476	1556	-238 -79 -194
ANISOU		CB	LEU LEU	26 26	23.674 1345	16.198 1522	46.285 1518	1.000 11.54 -75 -84 -202
ATOM	207	CG	LEU	26	23.242	17.638	46.019	1.000 12.42
ANISOU		CG	LEU	26	1199	1542	1978	-153 -167 - 4 0
ATOM	208	CD1	LEU	26	23.414	17.993	44.539	1.000 14.77
ANISOU			LEU	26	1428	1916	2270	43 131 4 0 1
ATOM	209		LEU	26	21.814	17.885	46.466	1.000 14.45
ANISOU ATOM	210		LEU	26	1384	2061	2047	264 -32 321
ANISOU	210	C C	LEU	26 26	23.979	14.209	47.780	1.000 12.93 -121 -486 - 107
ATOM	211	Ö	LEU	26	1360 23.011	1542 13.461	2011 48.008	-121 -486 - 107 1.000 13.78
ANISOU		ŏ	LEU	26	1660	1450	2125	-305 -426 - 51
ATOM	212	N	ARG	27	25.196	13.721	47.576	
ANISOU		N	ARG	27	1518	1729	2108	151 - 530 - 105
ATOM	213	CA	ARG	27	25.491	12.283	47.574	
ANISOU ATOM	213	CA CB	ARG ARG	27 27	2260 26.846	1690 12.122	1897 46.900	186 141 - 354 1.000 17.04
7 .1.6 J.M.					/n 4/16		75 000	

- 97 -

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ANISOU 214
           CB ARG 27
                       2259
                       2259 2356 1861 517 49 - 24
27.502 10.780 46.801 1.000 25.08
                                2356
                                               517 49 - 248
       215
ATOM
           CG ARG 27
ANISOU 215 CG ARG 27
ATOM 216 CD ARG 27
ANISOU 216 CD ARG 27
ATOM 217 NE ARG 27
                        3110
                               2837 3583
                                               1105 606 - 399
                        28.995 10.992 46.457 1.000 30.32
                        2976
                                3836
                                       4710
                                               1190 720 -1381
                        29.818 11.407 47.581 1.000 36.51
ANISOU 217
           NE ARG 27
                        3633
                                4937
                                       5301
                                               121 391 -1429
           CZ
                        30.988 12.019 47.560 1.000 38.07
MOTA
       218
               ARG 27
ANISOU 218
               ARG 27
           CZ
                        3334
                                5192
                                       5941
                                               364 661 -1776
           NH1 ARG 27
ATOM
       219
                       31.565 12.340 46.401 1.000 48.56
ANISOU 219
           NH1 ARG 27
                       4482
                               7688
                                               -1305 736 -1326
                                       6280
           NH2 ARG 27
ATOM
       220
                       31.606 12.328 48.701 1.000 40.23
           NH2 ARG 27
ANISOU 220
                       2891
                               6127
                                       6266
                                               457 717 - 2463
                       25.479 11.630 48.949 1.000 14.66
MOTA
       221
           С
               ARG
                    27
           С
ANISOU 221
               ARG
                    27
                        1720
                               1617
                                       2233
                                               135 -33 - 42
       222 0
ATOM
               ARG
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                        24.968 10.499 49.072 1.000 17.44
ANISOU 222 O
               ARG
                    27
                        1981
                               1533
                                       3114
                                               98 - 394 155
                       26.031 12.308 49.973 1.000 13.72
       223 N
MOTA
               ASP
                    28
ANISOU 223 N
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- 98 -

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ANISOU 249
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ATOM
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32 19.553
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MOTA
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ATOM
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ANISOU 267
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ATOM
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ANISOU 268
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CD2 TYR
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                TYR
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ANISOU 272
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MOTA
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- 99 -ANISOU 275 N LEU 34 1159 1265 1862 -210 -149 1 2 1 276 MOTA CA LEU 34 18.577 26.942 51.864 1.000 12.99 ANISOU 275 CALEU 34 1565 1444 1926 81 -478. 274 277 MOTA СВ LEU 34 17.757 26.420 50.682 1.000 13.96 ANISOU 277 СВ LEU 34 2007 1301 1995 -430 -459 3 2 1 273 MOTA CG LEU 34 17.990 27.112 49.334 1.000 13.81 ANISOU 278 CG LEU 34 2085 1322 1839 -331 -365 1 9 8 279 CD1 LEU ATOM 34 19.308 26.691 48.704 1.000 15.94 ANISOU 279 CD1 LEU 34 2123 1793 2140 -10 -313 6 0 7 280 ATOM CD2 LEU 16.818 26.799 48.411 1.000 16.36 34 ANISOU 280 CD2 LEU 34 2186 1837 2193 122 -721 1 3 4 281 MOTA С LEU 34 18.195 28.361 52.241 1.000 13.03 ANISOU 281 С LEU 34 1676 1418 1857 31 -643 218 ATOM 282 0 LEU 34 17.055 28.647 52.595 1.000 13.99 ANISOU 282 0 LEU 34 1690 1281 2344 140 -714 8 5 283 N MOTA THR 35 19.148 29.283 52.175 1.000 15.03 ANISOU 283 N THR 35 1837 1584 2288 -118 - 625 - 3284 CA THR 3 5 18.918 30.704 52.369 1.000 14.80 ANISOU 284 CATHR 35 1866 1560 2196 -169 -175 - 144 285 THR ATOM CB 35 20.013 31.366 53.232 1.000 15.65 ANISOU 285 CBTHR 35 2025 1719 2202 -149 -204 - 281 ATOM 286 OG1 THR 35 31.115 52.601 1.000 18.81 21.276 ANISOU 286 OG1 THR 3 5 1885 2679 -279 -229 - 728 2583 287 ATOM CG2 THR 35 20.138 30.811 54.622 1.000 18.84 ANISOU 287 CG2 THR 35 2523 2207 2427 -850 -510 1 5 5 ATOM 288 C THR 35 18.915 31.456 51.043 1.000 15.07 ANISOU 288 С THR 35 1904 1473 2348 -57 -283 - 70ATOM 289 0 THR 35 19.209 30.909 49.973 1.000 15.00 ANISOU 289 0 THR 35 - 2034 1520 2145 -215 -372 8 9 ATOM 290 N ASP 36 18.564 32.739 51.086 1.000 17.46 ANISOU 290 N ASP 36 2302 1366 -209 -766 - 120 2968 MOTA CA ASP 291 36 33.606 49.924 1.000 17.91 18.618 ANISOU 291 CAASP 36 2150 3063 1592 112 -660 8 6 292 ATOM CB ASP 36 20.063 33.845 49.471 1.000 17.91 ANISOU 292 СВ ASP 36 2153 1584 3067 84 - 587 - 42 293 ATOM CGASP 36 20.948 34.545 50.469 1.000 19.23 ANISOU 293 СG ASP 36 2575 2160 2571 -642 -324 1 8 1 ATOM 294 OD1 ASP 36 35.304 51.325 1.000 24.17 20.426 ANISOU 294 OD1 ASP 36 3055 2843 3284 152 -1013 -652 MOTA 295 OD2 ASP 3 5 22.199 34.355 50.412 1.000 21.00 ANISOU 295 OD2 ASP 36 2637 2772 2571 -382 -834 -393296 C MOTA ASP 36 17.783 33.038 48.784 1.000 18.20 ANISOU 296 C ASP 36 2402 1736 2779 -446 -390 1 9 1 33.063 47.629 1.000 18.98 ATOM 297 O ASP 36 18.222 ANISOU 297 O 36 ASP 2127 2022 3062 -464 -60 **-**252 32.547 49.077 1.000 17.22 ATOM 298 N CYS 37 16.593 ANISOU 298 N CYS 37 1873 2190 2479 63 - 350 - 1 ATOM 299 CA 31.945 48.043 1.000 15.98 CYS 37 15.730 ANISOU 299 CA CYS 37 1997 1590 2485 -81 -65 -184 ATOM 300 CB CYS 37 15.621 30.423 48.252 1.000 18.87 ANISOU 300 СB CYS 37 2112 1790 -114 -405 5 7 0 3268 301 MOTA SG CYS 37 14.753 29.917 49.759 1.000 19.42 ANISOU 301 SG CYS 37 2532 1683 -74 -230 3 2 2 3164 MOTA 302 С CYS 37 14.349 32.580 47.958 1.000 16.12 ANISOU 302 С CYS 37 1992 1669 2465 -175 -504 1 6 ATOM 303 0 CYS 37 13.483 32.032 47.253 1.000 20.60 ANISOU 303 0 CYS 37 2761 1769 3296 -241 -1333 5 1 MOTA 304 N GLY 38 33.714 48.617 1.000 17.89 14.125 ANISOU 304 N GLY 38 1847 1572 3381 209 -398 - 111ATOM 305 CAGLY 38 12.850 34.404 48.587 1.000 18.16 ANISOU 305 CAGLY 38 1608 2126 3164 141 -999 - 6

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 MOTA
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                  GLY 38
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                                      2574 3180
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 ATOM
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LEU 39
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 MOTA
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ATOM 314 C LEU 39

ANISOU 314 C LEU 39

ATOM 315 O LEU 39

ANISOU 315 O LEU 39

ATOM 316 N THR 40

ANISOU 316 N THR 40

ANISOU 316 N THR 40
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MOTA
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ANISOU 318
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ANISOU 319
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ANISOU 320
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ATOM
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ANISOU 321
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34.669 54.659 1.000 34.29
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ATOM
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             CG2 THR
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ANISOU 322
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                 ASP
             CG ASP
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ATOM
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ANISOU 329
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MOTA
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ANISOU 330 OD2 ASP
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ANISOU 332 CA
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ATOM
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ANISOU 333
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ANISOU 334
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ATOM
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ANISOU 335
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ATOM
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ANISOU 364 C
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ANISOU 365 O
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ATOM 372 CA LYS
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ATOM 373 C LYS
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ANISOU 374 O LYS
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ANISOU 375 CB LYS
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       424
                      54
                          -10.293 27.035
                                          56.619 1.000 23.32
ANISOU 424
            CD2 PHE
                      54
                          3482
                                  2802
                                          2577
                                                  -689 212 -858
MOTA
       425
            CE1 PHE
                      54
                          -12.719 28.291
                                         56.241 1.000 26.45
ANISOU 425
            CE1 PHE
                      54
                          3345
                                  3696
                                          3003
                                                  -1418 129 - 554
MOTA
            CE2 PHE
       426
                      54
                          -11.303 26.375
                                         55.921
                                                 1.000 25.65
ANISOU 426
            CE2 PHE
                      54
                          3750
                                  3815
                                          2182
                                                  -1404 607 -1005
ATOM
       427
            CZ
                 PHE
                      54
                          -12.522 27.013 55.725 1.000 26.17
ANISOU 427
            CZ
                 PHE
                      54
                          3433
                                  3830
                                          2679
                                                  -1829 298 - 813
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ANISOU 456

ANISOU 457

ATOM

457

458

CE1 HIS

NE2 HIS

NE2 HIS

HIS

57

57

PCT/GB98/03860 - 104 -MOTA 428 C PHE 54 -9.959 27.854 60.132 1.000 19.44 ANISOU 428 C PHE 54 2340 3430 1617 -834 319 -759 429 0 ATOM PHE -11.087 27.450 60.386 1.000 22.11 54 ANISOU 429 O PHE 54 2601 3066 -948 1018 -1466 2734 430 N ATOM PHE -8.882 27.166 60.448 1.000 20.59 55 ANISOU 430 N PHE 5 5 2728 3375 2728 3375 1720 -666 180 -611 -8.966 25.927 61.212 1.000 22.59 ATOM 431 CA PHE 55 ANISOU 431 CAPHE 55 3092 3671 1820 -728 381 -372ATOM 432 CB -7.579 25.360 61.478 1.000 21.93 PHE 55 ANISOU 432 CВ PHE 55 3163 3622 1549 -692 287 -158 433 ATOM CG -6.790 24.833 60.284 1.000 20.60 PHE 55 ANISOU 433 CG PHE 3034 2998 1793 -1004 365 -3 -7.352 24.526 59.057 1.000 18.72 55 -1004 365 - 375 434 ATOM CD1 PHE 55 ANISOU 434 CD1 PHE 55 2300 55 2300 3095 1717 -1078 586 -2 55 -5.430 24.615 60.385 1.000 18.06 -1078 586 - 271 ATOM 435 CD2 PHE ANISOU 435 CD2 PHE 55 3132 2490 1241 -926 128 -497 436 55 -5.609 24.037 58.014 1.000 18.92 ATOM CE1 PHE ANISOU 436 CE1 PHE 55 2455 2761 1971 -844 436 -542 MOTA 437 CE2 PHE 55 -4.672 24.124 59.352 1.000 18.58 ANISOU 437 ANISOU 437 CE2 PHE 55 3291 2606 1163 -478 63 -299 ANISOU 438 CZ PHE 55 -5.256 23.814 58.134 1.000 17.68 ANISOU 438 CZ PHE 55 -9.684 26.111 62.546 1.000 24.99 ANISOU 439 C PHE 55 -9.684 26.111 62.546 1.000 24.99 ANISOU 440 O PHE 55 3802 4943 2763 -1527 1314 -1102 ANISOU 441 N GLU 56 -9.330 27.144 63.311 1.000 23.65 ANISOU 441 N GLU 56 -9.330 27.144 63.311 1.000 23.65 ANISOU 442 CA GLU 56 -9.868 27.355 64.636 1.000 30.01 ANISOU 443 CB GLU 56 -8.998 28.333 65.436 1.000 30.01 ANISOU 443 CB GLU 56 -8.998 28.333 65.436 1.000 36.40 ANISOU 444 CG GLU 56 -8.998 28.333 65.436 1.000 36.40 ANISOU 444 CG GLU 56 -7.666 27.827 65.916 1.000 36.40 ANISOU 444 CG GLU 56 -7.666 27.827 65.916 1.000 41.89 ANISOU 444 CG GLU 56 -6.787 28.880 66.575 1.000 48.94 ANISOU 445 CD GLU 56 -6.787 28.880 66.575 1.000 48.94 ANISOU 445 CD GLU 56 6081 9310 3202 -2278 -73 -2062 ANISOU 446 OE1 GLU 56 -5.694 28.515 67.078 1.000 60.73 CE2 PHE 55 3291 2606 -478 63 - 299 1163 ANISOU 445 CD GLU 56 -6.787 28.880 66.575 1.000 48.94

ATOM 446 OE1 GLU 56 6081 9310 3202 -2278 -73 -2062

ANISOU 446 OE1 GLU 56 -5.694 28.515 67.078 1.000 60.73

ATOM 447 OE2 GLU 56 8034 12274 2769 -3208 -2335 2 6 6

ANISOU 447 OE2 GLU 56 8742 9338 4151 -2088 1096 -3951

ATOM 448 C GLU 56 8742 9338 4151 -2088 1096 -3951

ANISOU 448 C GLU 56 3764 4923 2941 -977 1967 -1271

ANISOU 449 O GLU 56 3764 4923 2941 -977 1967 -1271

ANISOU 449 O GLU 56 4384 5304 3690 -1136 2652 -1235

ANISOU 450 N HIS 57 -11.603 28.805 63.673 1.000 30.00

ATOM 450 N HIS 57 3730 4846 2823 -654 1684 -1582

ANISOU 451 CA HIS 57 3730 4846 2823 -654 1684 -1582

ANISOU 451 CA HIS 57 3853 5101 3778 -519 1673 -1911

ANISOU 452 CB HIS 57 3844 ANISOU 452 HIS CB 57 3844 5183 3664 -411 1546 - 2250 453 CG HIS -11.577 31.344 65.095 1.000 35.13 57 ANISOU 453 CG 4497 5409 HIS 57 3444 -505 1340 - 1992 454 CD2 HIS -10.361 31.946 65.071 1.000 35.26 57 CD2 HIS ANISOU 454 57 4837 5214 3345 -834 637 -1456 455 ND1 HIS 57 -11.819 31.021 66.411 1.000 40.52 ANISOU 455 ND1 HIS 57 6021 5885 3490 -1360 1474 - 2002 CE1 HIS 456 57 -10.798 31.410 67.151 1.000 42.28

6680 6066

3320

-9.902 31.970 66.362 1.000 41.69

57 -9.902 31.970 bb.362 1.000 41.69 57 6377 6133 3329 -1817 407 -1 57 -13.769 29.466 62.547 1.000 32.58

-1632 1099 -1772

-1817 407 -1148

- 105 -

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ANISOU 458 C
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                     57
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                                 5097
                                        4199
                                                -729 1723 - 2066
MOTA
       459 O
                HIS
                     57
                         -14.902 29.965 62.578 1.000 33.80
ANISOU 459 O
                HIS
                     57
                         3121
                                 5097 4625
                                                -731 1865 - 2565
MOTA
       460 N
                GLY
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                         -13.370 28.866 61.432 1.000 28.78
ANISOU 460 N
                GLY
                     58
                         2341
                                 4353
                                         3742
                                                -253 1341 - 1506
MOTA
       461
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ANISOU 461
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                                 3916
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                                                24 1298 -1173
MOTA
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ANISOU 462
           С
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                                 4357
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MOTA
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ANISOU 463 O
                GLY
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                                 4044
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       464 N
MOTA
                         -16.635 27.958 60.193 1.000 27.61
                SER
                     59
ANISOU 464 N
                SER
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                         2556
                                 3905
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ATOM
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                     59
ANISOU 465
            CA
               SER
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ATOM
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               SER
                     59
ANISOU 466
            CВ
                     59.
                SER
                               4574
                         2556
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ATOM
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                SER
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ANISOU 467
            OG SER
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                                 3742
                                         3547
                                                166
                                                      1729 - 867 .
           C
ATOM
       468
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                     59
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ANISOU 468
                SER
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                                 3990
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       469
ATOM
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ANISOU 469
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               SER
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ATOM
       470 N
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               GLU
ANISOU 470 N
                     60 2413 3900 3907 -69 1079 -
60 -18.699 23.684 59.359 1.000 26.98
               GLU
                                                      1079 - 853
       471 CA GLU
ATOM
ANISOU 471
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60 -19.646 22.681 60.001 1.000 39.11
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ATOM
       472
           CB GLU
ANISOU 472
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                     60 - 5393
               GLU
                              4393
                                       5075
                                                -1361 908 3 6 4
MOTA
       473
            CG
               GLU
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ANISOU 473
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               GLU
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                                                -977 1079 1219
ATOM
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            CD
               GLU
                    60
ANISOU 474
                        5714 6217 6503 -390 1207 8
-17.030 21.223 59.684 1.000 48.11
            CD
               GLU
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                    60
                                                -390 1207 8 7 7
ATOM
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                    60
ANISOU 475
            OE1 GLU
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                    60
                                 7545 5384
                                               709
                                                     366 1951
ATOM
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ANISOU 476
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                                 5742
                                        7000 1158 1550 - 1504
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ATOM
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               GLU
                    60
ANISOU 477 C
               GLU
                     60
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                        2829
ATOM
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               GLU
                    60
ANISOU 478 O
              {	t GLU}
                    60 2119
               GLU 60 2119 2980 4091 -202 741 -
ALA 61 -20.032 24.890 57.716 1.000 25.58
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MOTA
ANISOU 479 N
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ATOM
ANISOU 480 CA ALA 61 1838
                                 2999
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ATOM
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ANISOU 481
          CB ALA 61
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MOTA
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ANISOU 482
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ATOM
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ANISOU 484
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               GLU
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                                                     569 - 394
ATOM
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ANISOU 485
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               GLU
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                                 2603
                                        4188
                                                150 852 - 590
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ATOM
      486
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ANISOU 486
           CВ
               GLU
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                        2401
                                 2490
                                        4485
                                                91 1273 -828
ATOM
      487
           CG
               GLU
                    62
                        -17.641 29.636 56.356 1.000 25.19
ANISOU 487
           CG
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                                 2620
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                                                353 421 -685
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               GLU
                    62
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ATOM
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                                                                      62
                                                                               4832 2994 5584 863 109 -1327
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     ANISOU 490
                                        OE2 GLU
                                                                      62
     MOTA
                         491
                                        С
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                                                                      62
                                                                               2394 2421 3430 30 /84 - 3 / 3 - 15 .818 26 .218 53 .940 1 .000 19 . 44
     ANISOU 491
                                        С
                                                      GLU
                                                                      62
                                       O GLU
     ATOM
                          492
                                                                      62
    ANISOU 492 O GLU
                                                                               2095 2140 3153 -301 467 - 6
-16.184 25.308 55.972 1.000 20.08
                                                                      62
                                                                                                                                                        -301 467 -604
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                                                                      63
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63 -15.246 24.227 55.678 1.000 19.73
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CB LYS 63 -14.934 23.497 56.988 1.000 18.48
CB LYS 63 1803 2743 2476 -218 587
    ANISOU 494
                                                                                                                                                                         429 - 903
                         495
    ATOM
                                        CG LYS 63 2115 2332 2476 218 587 -8
    ANISOU 495
                                        CB LYS 63 1803
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    MOTA
                                        CG LYS 63 -13.840 21.21

CG LYS 63 2115 2332 2836 -296 325 -6

CD LYS 63 -13.839 23.651 59.290 1.000 26.23
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    ATCM
    ANISOU 497
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                                                   LYS 63 -12.753 24.383 60.068 1.000 27.75
LYS 63 3074 5008 2461 -1239 500 -1
                        498
    ATOM
                                        CE
    ANISOU 498
                                        CE
ANTISOU 498 CE LYS 63 3074 5008 461.530 1.000 34.95
ANTISOU 499 NZ LYS 63 -12.929 24.378 61.530 1.000 34.95
ANTISOU 500 C LYS 63 -15.789 23.304 54.586 1.000 17.52
ANTISOU 501 C LYS 63 -15.025 22.953 53.654 1.000 17.58 1.000 34.95
ANTISOU 501 C LYS 63 -15.025 22.953 53.654 1.000 17.58 1.000 34.95
ANTISOU 501 C LYS 63 -15.025 22.953 53.654 1.000 17.58 1.000 34.95
ANTISOU 501 C LYS 63 -15.025 22.953 53.654 1.000 17.58 1.000 34.95
ANTISOU 502 N ARG 64 -17.069 22.912 54.641 1.000 19.63 1.000 34.95
ANTISOU 502 N ARG 64 -17.618 22.041 53.595 1.000 19.00 19.00 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.000 34.
                                                                                                                                                         -1239 500 -1082
                                        NZ LYS 63 -12.929 24.378 61.530 1.000 34.95
NZ LYS 63 3177 7579 2524 -2594 840 -
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    ATOM
    ANISOU 499
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CB VAL 66 -12.775 25.151 50.951 1.000 17.29
ANISOU 519
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MOTA
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ANISOU 520
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                    66 1805
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MOTA
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           CG1 VAL
ANISOU 521
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                               1800
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           CG2 VAL
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MOTA
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           CG2 VAL
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                    66 2053 1996
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MOTA
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ATOM
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ANISOU 524 O
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MOTA
      525
           M
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                    67
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ANISOU 526
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              THR
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ATOM
           CВ
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           CB THR
                   67 1721
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           OG1 THR
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           OG1 THR
ANISOU 528
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                               1949
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ATOM
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ANISOU 529
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ATOM
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ANISOU 531 O THR
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MOTA
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ATOM
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ATOM
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MOTA
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ANISOU 539
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ANISOU 542 CG PRO
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72 1296 1581 1923 -46 328 -172 -6.418 13.805 49.549 1.000 17.83

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ANISOU 597
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              {	t GLY}
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ANISOU 598
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ANISOU 599 O
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ANISOU 600
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ATOM
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MOTA
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MOTA
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ANISOU 610
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ATOM 61: ANISOU 61: ATOM 62: ANISOU 62: ATOM 62: ANISOU 63: ANISOU	THREAD TH	78	.137 02 .853 69 .739 39 .299 70 .489 09 .685 33 .241 37	19.439 19.7053 19.7053 10.053 12.70	1629 76 1880 66 1880 66 154.66 88 158 66 158 66 158 66 158 67 158 67 158 67 158 67 158 67 158 67 158 77 158 77	-472 1.000 -508 1.000 -88 1.000 -1119 -1747 1.000 -1718 1.000 -1718 1.000 -1352 1.000 -1.000 -1.000 1.000 21.000 -1	22.91 06 -606 25.08 621 361 24.30 480 200 25.14 5-5 27.16 918 641 29.43 1260 173 38.31 1987 - 287 29.85 1307 - 264 25.58 -82 510 25.98 -55 424 26.28 407 841 28.19 799 - 544 29.83 270 181 25.34 -1220 158 27.00
ATOM 634 ANISOU 634 ATOM 635 ANISOU 635	O GLU CB GLU CB GLU CG GLU CG GLU	81 37 81 -7 81 35 81 -7 81 17	09 .685 33 .241 37	3520 9.861 2894 8.832 2915	3483 61.123 4906 60.098 4976	253 1.000 -770 1.000 284	799 - 544 29.83 270 181 25.34 -1220 158
		81 18 81 -8 81 34 81 -7 81 35 82 -4 82 35 82 -3 82 36	41 .120 44 .240 14 .988 68 .653	9.156 3405 10.240 3091 8.273 3384 9.974 3780 9.422 3278 8.150	58.649 5012 58.324 4413 57.814 4999 62.720 4430 62.959 4540	1.000 475 1.000 322 1.000 162 1.000 -65 1.000	27.00 -1887 - 456 28.81 -155791 31.31 352 100 31.00 -30 1484 30.29 -5151011 31.76

						- 111 -		
ANISOU		C	SER	82	3995	3241	4831	-102 -1104 8 4 7
ATOM ANISOU	642	0	SER	82	-4.313	7.728	61.397	1.000 34.01
ATOM	643	CB	SER SER	82 82	3193 -3.463	3794 9.167	5935	458 -1188 1 3 4
ANISOU		CB	SER	82	4687	3907	64.452 4606	1.000 34.74 -232 -979 9 7 1
ATOM	644	OG	SER	82	-2.360	8.305	64.681	1.000 41.53
ANISOU		OG	SER	82	4922	5366	5490	236 -1958 9 7 0
ATOM ANISOU	645 645	N N	GLY	91	-17.230		70.136	1.000 42.64
ATOM	646	CA	GLY	91 91	4516 -17.485	7599	4086	-2166 2340 - 427
ANISOU		CA	GLY	91	6666	7702	69.789 2697	1.000 44.91 -4311 -1561 5 6 5
MOTA	647	С	GLY	91	-16.227	11.662	69.452	1.000 38.67
ANISOU		C	GLY	91	5455	7587	1652	-2821 -274 - 159
ATOM ANISOU	648 648	0	$\operatorname{GLY} olimits$	91 91	-15.164 4241		70.040	1.000 32.45
ATOM	649	N	GLY	92	-16.332	4474	3616 68.474	-183 1152 - 439 1.000 31.97
ANISOU		N	GLY	92	3881	5904	2363	-1382 735 -571
ATOM	650	CA	GLY	91	-15.232	13.412	68.075	1.000 33.02
ANISOU ATOM	651	C A C	GLY GLY	92 92	4121	6150	2274	-1716 851 - 956
ANISOU		C	GLY	92	-15.223 2603	5046	66.572 2314	1.000 26.22 -885 741 -947
ATOM	652	O	GLY	92	-16.289		65.939	-885 741 -947 1.000 23.91
ANISOU		0	GLY	92	2490	3396	3198	-680 548 -567
ATOM ANISOU	653 653	N N	SER SER	93	-14.010		66.088	1.000 23.77
ATOM	654	CA	SER	93 93	2405 -13.801	3917	2708 54.690	-372 736 -560 1.000 23.41
ANISOU	654	CA	SER	93	2700	3292	2901	-386 970 -399
ATOM	655	C	SER	93	-12.410	13.852	64.240	1.000 24.26
ANISOU ATOM	655 656	C 0	SER SER		2547	3908	2763	-286 833 -224
ANISOU		0	SER	93 93	-11.497 3401	3536	65.089 3346	1.000 27.06 630 92 - 386
ATOM	657	СB	SER	93	-13.966	15.795	64.467	630 92 - 386 1.000 25.71
ANISOU		CB	SER	93	2811	3225	3735	-576 271 -506
ATOM ANISOU	658	OG OG	SER SER	93		16.158	63.150	1.000 28.14
ATOM	659	N	TYR	93 94	2694 -12.254	3713	4284 62.949	-373 290 517 1.000 24.24
ANISOU		N	TYR	94	2786	3320	3104	-204 791 -817
ATOM	660	CA	TYR	94	-10.878	13.262	62.498	1.000 23.94
ANISOU ATOM	661	CA C	$ ext{TYR}$	94	3089	2502	3505	95 1112 - 683
ANISOU		C	TYR	94 94	-10.017 2601	2657	62.584 4312	1.000 25.19 147 737 -625
ATOM	662	Ō	TYR	94	-8.786	14.421	62.694	147 737 - 625 1.000 30.11
ANISOU		0	TYR	94	2617	3095	5726	307 760 3 6
ATOM ANISOU	663	CB CB	TYR	94	-10.800		61.098	1.000 25.64
ATOM	664	CG	$ ext{TYR}$	94 94	3566 -11.600	2910	3267 60.876	-293 1331 - 525
ANISOU	664	CG	TYR	94	3359	2768	2697	1.000 23.22 -69 784 - 274
ATOM	665	CD1	TYR	94	-12.451		59.777	1.000 26.01
ANISOU ATOM	666	CD1 CD2	TYR	94	4410	2730	2741	499 353 -543
ANISOU		CD2	TYR TYR	94 94	-11.564 3117	10.252 2866	61.635 3297	1.000 24 . 42
ATOM	667	CE1	TYR	94	-13.243	10.407	59.443	73 458 - 1 4 1.000 28.75
ANISOU		CE1	TYR	94	4559	3328	3037	434 140 - 1370
ATOM ANISOU	668 668	CE2	TYR TYR	94	-12.375		61.305	1.000 26.47
ATOM	669	CE2	TYR	94 94	4707 -13.209	2585	2764	-220 1227 - 718 1.000 29.70
ANISOU	669	CZ	TYR	94	5641	3518	60.212 2125	-1172 1103 - 1447
ATOM	670	OH	TYR	94	-14.059	8.281	59.730	1.000 34.02
ANISOU ATOM	671	ОН И	TYR SER	94	3079	3962	5886	-423 1593 - 2638
ANISOU		N	SER	95 95	-10.628 2460	15.714 2497	62.561 3632	1.000 22.61 -54 59 - 338
				- 0	- 100	~ 4) /	J U J Z	-74 73 - 2 2 0

ATOM 672 CA SER 95 -9.924 16.975 62.750 1.000 22.54 ANISOU 672 CA SER 95 2257 2603 3706 -120 -301 4 6 ANISOU 673 C SER 95 -9.370 17.106 64.163 1.000 23.58 ATOM 674 O SER 95 1811 3478 3671 -521 -88 -85 ANISOU 674 O SER 95 -8.623 18.034 64.481 1.000 26.53 ATOM 675 CB SER 95 -10.838 18.177 62.478 1.000 27.58 ANISOU 675 CB SER 95 3657 2556 4264 365 -379 2 8 ANISOU 676 OG SER 95 -11.506 18.093 61.242 1.000 39.40 ATOM 677 N ASP 96 -9 712 16 184 421 900 -1445 144	
ANISOU 677 N ASP 96 2579 3688 3248 -3999 277 -232 ANISOU 678 CA ASP 96 -9.228 16.317 66.422 1.000 24.42 ANISOU 679 C ASP 96 -7.735 16.050 66.501 1.000 24.45 ANISOU 679 C ASP 96 2597 3228 3466 -471 162 -383 ANISOU 680 O ASP 96 2597 3228 3466 -471 162 -383 ANISOU 681 CB ASP 96 2557 3228 3466 -471 162 -383 ANISOU 681 CB ASP 96 2556 4047 3370 -170 160 -798 ANISOU 681 CB ASP 96 -9.952 15.334 366 -472 160 -798 ANISOU 682 CG ASP 96 -11.411 15.605 67.606 1.000 24.97 ANISOU 682 CG ASP 96 -11.935 16.723 67.304 1.000 24.97 ANISOU 683 ODI ASP 96 -11.935 16.723 67.304 1.000 24.97 ANISOU 684 OD2 ASP 96 -11.935 16.723 67.304 1.000 23.06 ANISOU 685 N TYR 97 -7.254 15.226 65.581 1.000 32.65 ANISOU 685 N TYR 97 -7.254 15.226 65.581 1.000 22.21 ANISOU 687 CA TYR 97 -5.026 15.828 64.743 1.000 22.21 ANISOU 688 O TYR 97 -5.026 15.828 64.743 1.000 22.306 ANISOU 688 O TYR 97 -5.026 15.828 64.743 1.000 22.307 ANISOU 689 CB TYR 97 -5.025 15.828 64.743 1.000 22.306 ANISOU 689 CB TYR 97 -5.026 15.828 64.743 1.000 23.06 ANISOU 689 CB TYR 97 -5.025 15.828 64.743 1.000 23.06 ANISOU 689 CB TYR 97 -5.585 13.451 65.035 1.000 22.21 ANISOU 689 CB TYR 97 -5.585 13.451 66.285 1.000 30.19 ANISOU 690 CG TYR 97 -3.591 16.691 66.285 1.000 30.19 ANISOU 690 CG TYR 97 -3.511 12.691 66.285 1.000 32.77 ANISOU 690 CG TYR 97 -3.511 12.691 66.285 1.000 32.77 ANISOU 690 CG TYR 97 -3.511 12.691 66.285 1.000 32.77 ANISOU 690 CG TYR 97 -3.511 12.691 66.285 1.000 32.77 ANISOU 690 CG TYR 97 -3.511 12.691 66.324 1.000 32.77 ANISOU 690 CG TYR 97 -3.511 12.691 66.325 1.000 32.77 ANISOU 690 CG TYR 97 -3.511 12.691 66.325 1.000 32.77 ANISOU 690 CG TYR 97 -2.178 12.294 66.324 1.000 32.77 ANISOU 690 CG TYR 97 -2.178 12.294 66.324 1.000 32.77 ANISOU 690 CG TYR 97 -2.178 12.294 66.324 1.000 32.77 ANISOU 690 CG TYR 97 -2.178 12.294 66.324 1.000 32.77 ANISOU 690 CG TYR 97 -2.178 12.294 66.324 1.000 32.77 ANISOU 690 CG TYR 97 -2.178 12.294 66.324 1.000 32.77 ANISOU 690 CG TYR 97 -2.178 12.294 66.324 1.000 32.77 ANISOU 690 CG TYR 97 -2.178 12.294 66.324 1.000 32.77 ANISOU 690 CG	5 11 142 142 163 8 2 2
ANISOU 696 OH TYR 97 2572 5373 8264 1161 764 1277 ANISOU 697 CB SER 98 -3.465 16.575 62.134 1.000 23.20 ATOM 698 OG SER 98 -3.632 15.649 61 078 1 000 26 42	

- 113 -ANISOU 702 CA SER 98 2430 2687 2982 133 153 294 ATOM 703 N MET 99 -5.307 18.891 61.148 1.000 18.68 ANISOU 703 N MET 99 2392 2722 1984 -978 -366 1 0 1 CA MET 99 -6.047 19.560 60.075 1.000 17.84 ATOM 704 ANISOU 704 MET 99 2431 CA2620 1726 -945 -212 - 17 MOTA 705 CB MET 99 -6.819 20.779 60.585 1.000 19.71 ANISOU 705 CB MET 99 2348 2968 2173 -679 25 6 4 ATOM 706 CG MET 99 -8.052 20.392 61.374 1.000 23.68 ANISOU 706 CG MET 99 2360 3055 3582 -504 393 489 99 -9.031 21.821 61.911 1.000 22.33 ATOM 707 SD MET ANISOU 707 SD MET 99 2569 3383 2534 -522 170 -120 708 ATOM CE MET 99 -8.148 22.225 63.419 1.000 36.98 ANISOU 708 CE MET 99 6485 4165 3401 -225 -1904 - 23 709 MOTA C MET 99 -5.070 19.954 58.973 1.000 17.19 ANISOU 709 С MET 99 2269 2488 1776 -960 -194 - 201 710 0 ATOM MET 99 -3.964 20.341 59.324 1.000 16.93 ANISOU 710 O MET 99 1932 2583 1919 -367 -208 -241100 -5.486 19.864 57.715 1.000 20.00 MOTA 711 N CYS ANISOU 711 N CYS 100 3178 2683 1739 -1753 -358 1 6 6 712 CA CYS ATOM 100 -4.645 20.181 56.554 1.000 16.64 ANISOU 712 CA CYS 100 2213 2294 1817 -924 -563 4 6 8 MOTA 713 100 -4.291 18.893 55.813 1.000 17.74 CB CYS ANISOU 713 CB 100 2161 CYS 2407 2174 560 -765 1 0⁻53 MOTA 714 SG CYS 100 -3.035 18.928 54.552 1.000 33.56 ANISOU 714 SG CYS 100 5244 3511 3997 1509 6 0 1 414 715 C MOTA CYS 100 -5.347 21.121 55.590 1.000 13.48 ANISOU 715 C CYS 100 1879 1415 1829 -68 240 - 91716 O CYS ATOM 100 -6.585 21.127 55.496 1.000 14.49 ANISOU 716 O CYS 100 1880 1952 1673 -497 -57 717 N ATOM 101 -4.589 21.921 54.852 1.000 13.35 TYR ANISOU 717 N TYR 101 1721 1677 1673 -254 -78 4 9 718 CA TYR 101 -5.016 22.753 53.755 1.000 10.27
718 CA TYR 101 926 1498 1477 -15 -141 -231
719 CB TYR 101 -5.102 24.265 54.124 1.000 13.60
719 CB TYR 101 1626 1513 2027 -48 322 -23 ATOM ANISOU 718 ATOM ANISOU 719 322 - 236 ATOM 720 CG TYR 101 -5.498 25.025 52.863 1.000 17.31 TYR ANISOU 720 CG 101 2373 1509 2694 -158 -103 1 9 3 ATOM 721 CD1 TYR 101 -6.815 25.068 52.519 1.000 16.38 ANISOU 721 CD1 TYR 101 2464 752 3006 190 -227 5 5 722 CE1 TYR ATOM 101 -7.307 25.715 51.412 1.000 17.01 101 2755 714 2993 -86 -416 12 ANISOU 722 CE1 TYR 714 2993 -86 -416 122 101 -4.616 25.679 52.012 1.000 19.51 101 3032 1533 2847 -1143 -594 4 7 5 101 -5.065 26.321 50.872 1.000 20.96 CD2 TYR ATOM 723 ANISOU 723 CD2 TYR 724 MOTA CE2 TYR CE2 TYR 101 2802 1949 3211 238 112 769 101 -6.414 26.334 50.568 1.000 22.78 ANISOU 724 CZ TYR ATOM 725 ANISOU 725 101 3238 2291 3126 -1228 -919 6 2 4 101 -6.875 26.986 49.442 1.000 23.10 CZTYR 726 OH TYR MOTA ANISOU 726 OH TYR 101 3141 3112 2522 -14 -129 4 2 9 101 -4.041 22.518 52.596 1.000 11.25 MOTA 727 С TYR ANISOU 727 C TYR ATOM 728 O TYR ANISOU 728 O TYR ATOM 729 N SER ANISOU 729 N 102 1355 SER 1279 1611 -220 145 -263 102 -3.752 21.802 50.235 1.000 10.46 ATOM 730 CA SER ANISOU 730 CA SER 102 1144 102 1144 1263 1568 62 -1 -125 102 -4.027 20.343 49.908 1.000 13.46 ATOM 731 CB SER ANISOU 731 СВ SER 102 1668 1212 2234 324 105 - 301 102 -3.723 19.487 51.025 1.000 16.42 MOTA 732 OG SER ANISOU 732 OG SER 102 2291 1313 2637 -122 -43 9 6

- 114 -ATOM 733 C SER 102 -4.046 22.668 49.008 1.000 11.74 ANISOU 733 C SER 102 1346 1500 1614 18 -39 - 10 1500 1614 18 - 39 - 10 734 O SER 23.148 48.784 1.000 12.84 1410 1988 90 -66 249 ATOM 102 -5.148 ANISOU 734 O SER 102 1480 ATOM 735 N MET 103 -3.004 22.871 48.187 1.000 12.33 ANISOU 735 N MET 103 1554 1722 1409 -262 -10 -246103 -3.188 23.603 46.938 1.000 12.92 103 1663 1681 1565 22 47 - 70 ATOM 736 CA MET ANISOU 736 CA MET 103 -3.215 25.122 47.179 1.000 17.51 103 2439 1634 2579 -363 812 -ATOM 737 CB MET ANISOU 737 CB MET -363 812 -44 CG MET 103 -1.929 25.808 47.549 1.000 20.07 ATOM 738 ANISOU 738 CG MET 103 2509 1470 3646 -538 688 376 739 SD MET 103 -2.136 27.614 47.689 1.000 18.10 ATOM ANISOU 739 ANISOU 739 SD MET 103 2235 1665 2975 -3 -334 -35
ATOM 740 CE MET 103 -2.365 28.068 45.991 1.000 18.09
ANISOU 740 CE MET 103 2319 1457 3098 -187 -718 -2
ATOM 741 C MET 103 -2.152 23.221 45.892 1.000 12.57
ANISOU 741 C MET 103 1420 1837 1519 119 -53 2
ATOM 742 O MET 103 -1.120 22.573 46.175 1.000 12.57
ANISOU 742 O MET 103 1094 1891 1792 -155 -165 2
ATOM 743 N GLY 104 -2.418 23.650 44.655 1.000 12.83
ANISOU 743 N GLY 104 1493 1958 1422 237 -124 -2
ATOM 744 CA GLY 104 -1.533 23.459 43.513 1.000 12.65 SD MET 103 2235 1665 2975 -3 -334 -352 -187 -718 -214
 103
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ANISOU 743 N GLY 104 1493 1958 1422 237 -124 - 34

ATOM 744 CA GLY 104 -1.533 23.459 43.513 1.000 12.65

ANISOU 744 CA GLY 104 1075 2188 1544 -93 -37 242

ATOM 745 C GLY 104 -1.624 24.622 42.542 1.000 14.36

ANISOU 745 C GLY 104 1909 1985 1561 -265 -294 142

ATOM 746 O GLY 104 -2.033 25.700 42.967 1.000 15.69

ANISOU 746 O GLY 104 1628 2273 2060 163 -197 2 1 3

ATOM 747 N THR 105 -1.242 24.397 41.276 1.000 14.52

ANISOU 747 N THR 105 1829 2182 1504 -59 -375 3 1 9

ATOM 748 CA THR 105 -1.218 25.452 40.279 1.000 15.27

ANISOU 748 CA THR 105 1977 2223 1603 -105 -363 3 6 5 ANISOU 748 CA THR 105 1977 2223 1603 -105 -363 3 6 5
ATOM 749 CB THR 105 -0.359 25.083 39.039 1.000 15.61
ANISOU 749 CB THR 105 1936 2122 1873 -37 -106 5 5 4
ATOM 750 OG1 THR 105 -0.884 23.876 38.446 1.000 16.16
ANISOU 750 OG1 THR 105 1738 2260 2140 217 -285 1 5 1
ATOM 751 CG2 THR 105 1.092 24.882 39.369 1.000 17.47
ANISOU 751 CG2 THR 105 1918 2871 1847 -293 -227 5 2 7
ATOM 752 C THR 105 -2.603 25.828 39.755 1.000 14.73
ANISOU 753 C THR 105 1989 1694 1913 122 ATOM 752 C THR 105 -2.603 25.626 35.733 1.000 12...5

ANISOU 752 C THR 105 1989 1694 1913 122 -340 19

ATOM 753 O THR 105 -2.730 26.921 39.174 1.000 19.91

ANISOU 753 O THR 105 2579 2355 2632 23 -437 1004

ATOM 754 N ALA 106 -3.587 24.960 39.913 1.000 16.57

ANISOU 754 N ALA 106 1836 2413 2047 2 -260 661

ATOM 755 CA ALA 106 -4.975 25.167 39.465 1.000 14.94

ANISOU 755 CA ALA 106 1975 1904 1798 105 -456 36

ATOM 756 CB ALA 106 -5.054 24.945 37.965 1.000 17.75

ANISOU 756 CB ALA 106 -5.054 24.945 37.965 1.000 17.75

ANISOU 757 C ALA 106 -5.942 24.251 40.222 1.000 16.26

ANISOU 757 C ALA 106 1710 2174 2293 327 -127 4 9 23 -437 1004 -456 3 6 5 -201 - 3 2 ALA 106 1710 2174 2293 327 -127 4 9 1 758 O ALA 106 -5.498 23.398 41.013 1.000 14.57 ATOM . ANISOU 758 O ALA 106 1622 213 -21 3 3 7 1971 1945 759 N ASP ATOM 107 -7.253 24.410 40.008 1.000 16.71 ANISOU 759 N ASP 107 1768 2096 2485 540 -22 3 0 4 760 CA ASP 107 -8.310 23.638 40.633 1.000 16.10 ATOM ANISOU 760 CA ASP 107 1696 2246 2175 51 - 485 - 14 107 -8.231 22.171 40.211 1.000 17.09 ATOM .761 CB ASP ANISOU 761 CB ASP 107 1299 2385 2808 144 -203 - 399
 107 1299
 2385
 2808
 144
 -203 - 3

 107 -8.418
 21.966
 38.720
 1.000 21.54

 107 2385
 2894
 2906
 84 -317 - 72

 107 -9.452
 22.445
 38.189
 1.000 23.92
 ATOM 762 CG ASP ANISOU 762 CG ASP 2906 84 -317 -722 ATOM 763 OD1 ASP

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ANISOU ATOM	763 764		ASP		3447	2970	2672	698 -753 - 772
ANISOU			ASP ASP	107	-7.563 2496	21.311	38.080	
ATOM	765	C	ASP		-8.285	4004 23.785	2954 42.160	105 244 -679
ANISOU		С	ASP	107	1261	1918	2201	1.000 14.16 237 -447 153
ATOM	766	0	ASP	107	-8.507	22.850	42.936	1.000 16.67
ANISOU ATOM	767	O N	ASP	107		1927	2390	-189 -193 9 7
ANISOU		N	ASN ASN		-8.027 2093	25.020 1866	42.598	1.000 15.34
ATOM	768	CA	ASN		-7.967	25.314	1870 44.031	82 51 2 3 9
ANISOU		CA	ASN	108	1479	1823	1898	1.000 13.68 153 107 257
ATOM ANISOU	769	CB CB	ASN		-6.925	26.420	44.272	1.000 15.60
ATOM	770	CG	ASN ASN		1593 -5.516	2026 25.942	2309	16 267 - 98
ANISOU		CG	ASN	108		23.942	43.963 2142	1.000 15.23 5 -53 2
ATOM	771		ASN	108	-5.086	24.932	44.505	1.000 15.40
ANISOU ATOM	771 772		ASN ASN			2442	1998	-5 -239 188
ANISOU			ASN	108	-4.823 1593	26.678 2198	43.094	1.000 16.96
ATOM	773	C	ASN		-9.310	25.708	2652 44.642	339 393 222 1.000 14.55
ANISOU		C	ASN	108	1471	1937	2120	261 191 5 2 6
ATOM ANISOU	774 774	0	ASN	108	-10.222		43.958	1.000 16.89
ATOM	775	N .	ASN LEU	108	1861 -9.412	2336 25.512	2219	716 -109 1 4
ANISOU		N	LEU	109	1458	1648	45.954 1994	1.000 13.42 179 130 9
ATOM	776	CA	LEU	109	-10.602	25.796	46.769	1.000 13.53
ANISOU ATOM	777	CA CB	LEU LEU		1094	2122	1923	-52 -86 -256
ANISOU		CB	LEU	109	-11.187 1382	24.499 1959	47.331 2169	1.000 14.50
ATOM	778	CG	LEU	109	-11.580	23.383	46.370	119 455 - 468 1.000 15.21
ANISOU ATOM	778 779	CG CD1	LEU	109	1593	1785	2403	235 63 - 342
ANISOU		CD1		109	-11.931 2460	22.083 1674	47.089	1.000 18.26
ATOM	780	CD2	LEU		-12.780	23.783	2806 45.529	382 -414 - 9 4 1.000 22.36
ANISOU		CD2		109	3055	2391	3052	44 -1155 2 8 8
ATOM ANISOU	781 781	C	LEU LEU	109	-10.203		47.840	1.000 13.54
ATOM	782	0	LEU		1179 -9.416	1989 26.428	1979 48.717	76 -116 -259
ANISOU		0	LEU	109	2196	2210	1730	1.000 16.15 -52 -366 3 2
ATOM ANISOU	783	N	PHE	110	-10.706	28.025	47.786	1.000 16.11
ATOM	784	N CA	PHE PHE		1369	2042	2709	105 -118 - 288
ANISOU	784	CA	PHE	110	-10.298 1626	1801	48.732 3050	1.000 17.05 -116 259 - 362
ATOM	785	CB	PHE	110	-9.660	30.259	47.991	1.000 17.94
ANISOU ATOM	785 786	CB CG	PHE PHE	110	1423	2366	3027	-290 228 -129
	786	CG	PHE	110	-8.425 1702	29.972 2650	47.165	1.000 20.32
ATOM	787	CD1	PHE	110	-7.257	29.598	3368 47.793	-176 459 -385 1.000 20.35
ANISOU ATOM	787 788	CD1	PHE	110	1885	2462	3387	461 573 - 707
ANISOU		CD2 CD2	DHE	110	-8.405 2073	30.110	45.789	1.000 20.31
ATOM	789	CE1	PHE		-6.102	2226 29.347	3419 47.065	512 712 - 264 1.000 19.49
	789	CE1	PHE	110	1958	2116	3332	176 749 - 631
ATOM ANISOU	790 790	CE2	PHE	110	-7.288	29.846	45.050	1.000 20.65
ATOM	791	CE2 CZ		110	2158 -6.118	2094	3596	758 724 - 321
ANISOU	791	CZ.	PHE	110	1925	29.496 2131	45.694 3327	1.000 19.43 219 542 - 780
ATOM	792	C	PHE	110	-11.495	29.556	49.538	1.000 17.08
ANISOU ATOM	792 793	C 0	PHE	110	1774	1806	2911	-74 414 -111
ANISOU		0	PHE PHE	110	-12.562 1849	29.792 2577	48.929	1.000 21.26
		_			-043	2311	3650	405 178 -448

- 116 -794 ATOM М PRO 111 -11.406 29.717 50.851 1.000 19.41 ANISOU 794 N PRO 111 2279 2110 2985 -386 519 -314 795 ATOM CDPRO 111 -10.278 29.322 51.705 1.000 19.20 ANISOU 795 CDPRO 111 2773 1880 2640 -417 255 -514 796 ATOM CAPRO 111 -12.549 30.252 51.604 1.000 21.47 ANISOU 796 CAPRO 111 3026 1924 3206 -50 728 -635 797 ATOM СВ PRO 111 -12.167 30.007 53.055 1.000 23.63 ANISOU 797 CB PRO 111 3789 2054 3137 334 776 - 575 798 ATOM CG PRO 111 -10.775 29.535 53.100 1.000 22.33 ANISOU 798 CG 111 2767 PRO 2908 2809 -1006623 - 414MOTA 799 С 111 -12.828 31.739 51.433 1.000 23.88 PRO ANISOU 799 C 111 3139 PRO 2049 3887 79 -142 -479 800 111 -13.919 32.194 51.834 1.000 26.77 ATOM 0 PRO ANISOU 800 0 PRO 111 3800 3555 2818 992 -91 -397 ATOM 801 N SER 112 -11.906 32.517 50.872 1.000 25.19 ANISOU 801 SER 112 3514 2269 3788 -247 -856 2 8 2 ATOM 802 CASER 112 -12.300 33.919 50 631 1.000 26.43 ANISOU 802 CASER 112 2654 2655 4734 496 1364 4 5 6 ATOM 803 112 -12.506 34.712 51.912 1.000 33.37 CB SER ANISOU 803 CВ SER 112 3122 3663 5895 172 2582 - 510 MOTA 804 OG SER 112 -11.322 34.719 52.688 1.000 36.94 ANISOU 804 OG SER 112 6530 2154 5351 1399 206 - 415 ATOM 805 С 112 -11.262 34.587 49.723 1.000 26.62 SER ANISOU 805 C 112 2613 SER 2546 4956 1021 1668 651 MOTA 806 0 112 -10.219 34.029 49.414 1.000 22.81 SER ANISOU 806 0 SER 112 2241 2782 3645 800 837 - 400 ATOM 807 N GLY 113 -11.570 35.802 49.279 1.000 28.93 ANISOU 807 N 113 2937 GLY 2947 5108 1008 1175 1198 MOTA 808 CAGLY 113 -10.659 36.478 48.365 1.000 30.79 ANISOU 808 CAGLY 113 2992 3606 5102 381 798 1400 ATOM 809 C GLY 113 -9.362 36.829 49.070 1.000 31.83 ANISOU 809 C GLY 113 3297 3919 4878 262 897 528 ATOM 810 0 GLY 113 -8.294 36.790 48.459 1.000 25.85 ANISOU 810 0 GLY 113 2920 2317 4585 857 450 - 203 MOTA 811 N ASP 114 -9.479 37.145 50.365 1.000 29.56 ANISOU 811 114 3487 N ASP 2877. 4868 866 1104 7 6 0 ATOM 812 CAASP 114 -8.257 37.463 51.122 1.000 26.15 ANISOU 812 CA114 3189 ASP 2680 4066 1028 1584 5 4 2 37.937 52.526 1.000 33.81 MOTA 813 CB ASP 114 -8.628 ANISOU 813 114 5580 CB ASP 2697 4569 1774 1691 - 240 ATOM 814 CG ASP 114 -7.904 39.232 52.840 1.000 40.77 ANISOU 814 CG ASP 114 6798 3734 4960 719 693 - 248 ATOM 815 OD1 ASP 114 -8.330 40.277 52.295 1.000 48.61 ANISOU 815 OD1 ASP 114 6014 2534 9920 1703 931 - 913 ATOM 816 OD2 ASP 39.178 53.622 1.000 54.35 114 -6.932 ANISOU 816 OD2 ASP 114 5258 7609 7783 -868 495 1602 MOTA 817 C ASP 114 -7.310 36.281 51.231 1.000 23.05 ANISOU 817 С ASP 114 2621 2102 4033 444 1874 3 4 0 ATOM 818 0 ASP 114 -6.111 36.371 50.955 1.000 22.05 ANISOU 818 0 ASP 114 2423 2277 3677 131 1411 - 461 ATOM 819 Ν PHE 115 -7.854 35.160 51.637 1.000 23.21 ANISOU 819 N PHE 115 2945 1890 3984 -130 1293 - 228 ATOM 820 PHE CA 115 -7.120 33.896 51.690 1.000 19.93 ANISOU 820 PHE CA115 2562 1908 3102 -1.98 655 -294115 -8.085 32.792 52.157 1.000 19.49 ATOM 821 CB PHE ANISOU 821 PHE CB 115 2378 1754 3275 64 881 - 314 ATOM 822 CG PHE 115 -7.523 31.445 52.540 1.000 17.25 ANISOU 822 CG PHE 115 2053 1589 2912 -56 348 -695 ATOM 823 CD1 PHE 115 -7.637 30.951 53.833 1.000 19.00 ANISOU 823 CD1 PHE 115 2728 1539 2950 73 496 - 683 ATOM 824 CD2 PHE 115 -6.868 30.634 51.615 1.000 17.88

- 117 -ANISOU 824 CD2 PHE 115 1933 7 298 -810 1931 2927 825 CE1 PHE 115 -7.100 29.711 54.163 1.000 20.25 ANISOU 825 CE1 PHE 115 2825 1825 3042 317 341 - 57529.412 51.955 1.000 19.11 826 CE2 PHE 115 -6.338 115 1865 ANISOU 826 CE2 PHE 2158 3237 336 351 -885 827 28.936 53.233 1.000 19.39 ATOM CZ PHE 115 - 6.452ANISOU 827 CZ115 2068 PHE 1910 3390 320 248 - 669 MOTA 828 C 115 -6.506 PHE 33.624 50.327 1.000 17.86 ANISOU 828 C PHE 115 1964 1945 2878 61 344 1 6 829 0 ATOM PHE 115 -5.324 33.315 50.271 1.000 17.34 ANISOU 829 O PHE 115 1868 2107 2613 -132 179 157 33.683 49.263 1.000 18.21 2107 2613 830 N ATOM GLU 116 -7.310 ANISOU 830 N GLU 116 1921 1934 3065 547 281 6 2 831 CA GLU 33.387 47.907 1.000 19.99 MOTA 116 -6.848 ANISOU 831 CAGLU 116 2128 2618 2851 81 231 2 2 2 832 CB 116 -7.968 33.605 46.884 1.000 18.61 MOTA GLU GLU ANISOU 832 CВ 116 2058 1952 3060 231 244 270 833 MOTA CG GLU 116 -7.396 33.378 45.482 1.000 18.61 ANISOU 833 CG GLU 116 1813 2288 2971 295 -32 - 33 MOTA 834 CD GLU 116 -8.442 33.230 44.412 1.000 22.40 ANISOU 834 CD GLU 116 1908 3193 3410 -122 -278 - 91116 -9.654 33.272 44.678 1.000 30.82 ATOM 835 OE1 GLU OE1 GLU ANISOU 835 116 1793 4465 5452 273 -414 - 24OE2 GLU MOTA 836 116 -8.085 33.063 43.225 1.000 30.24 ANISOU 836 OE2 GLU 116 3333 5132 3026 382 -658 3 2 7 MOTA 837 C 116 -5.620 34.211 47.535 1.000 18.82 GLU 116 2090 ANISOU 837 С GLU 2069 2990 294 119 487 MOTA 838 0 GLU 116 -4.605 33.701 47.049 1.000 17.41 116 2228 117 -5.660 ANISOU 838 0 GLU 1780 2606 45 259 282 ATOM 839 N ARG 35.508 47.777 1.000 21.02 ANISOU 839 N ARG 117 2313 2185 3487 408 220 9 0 840 117 -4.560 CAARG 36.420 47.431 1.000 21.35 ANISOU 840 CA ARG 117 2337 1800 3976 466 147 ATOM 841 C 117 -3.291 ARG 36.054 48.192 1.000 20.52 ANISOU 841 С ARG 117 2292 2124 3380 353 288 ATOM 842 0 117 -2.186 ARG 35.969 47.636 1.000 18.96 ANISOU 842 0 ARG 117 2223 1664 3316 138 318 231 ATOM 843 CB 117 -4.971 ARG 37.885 47.693 1.000 25.59 ANISOU 843 CB ARG 117 3237 1900 4587 929 1882 6 3 2 844 ATOM CG ARG 117 -3.881 38.908 47.478 1.000 32.57 ANISOU 844 CG ARG 117 5212 1925 5237 -281 1083 6 2 3 ATOM 845 CDARG 117 -4.325 40.323 47.859 1.000 36.56 ANISOU 845 CDARG 117 6009 2157 5724 149 1774 6 6 3 MOTA 846 ARG 117 -5.162 40.335 49.056 1.000 44.43 ΝE ANISOU 846 NE ARG 117 7200 3742 5940 -96 2344 - 15ATOM 847 ARG CZ117 -4.763 40.501 50.306 1.000 45.48 ANISOU 847 CZARG 117 6422 4804 6054 -370 2388 - 283 ATOM 848 NH1 ARG 117 -3.484 40.683 50.619 1.000 53.21 ANISOU 848 NH1 ARG 117 6867 6451 6900 -2543 2487 3 5 4 ATOM 849 117 -5.647 40.487 51.301 1.000 50.00 NH2 ARG ANISOU 849 117 6265 NH2 ARG 6511 6220 224 2433 - 1534 ATOM 850 NILE 118 -3.439 35.832 49.493 1.000 19.30 ANISOU 850 N ILE 118 2275 1838 3221 128 407 -645 MOTA 851 CAILE 118 -2.275 35.527 50.331 1.000 18.25 ANISOU 851 CAILE 118 2376 1745 2811 78 530 - 449 MOTA 852 CB ILE 118 -2.665 35.597 51.820 1.000 18.24 ANISOU 852 CB ILE 118 2201 1726 3003 346 906 -34.851 52.732 1.000 18.49 346 906 - 306 CG2 ILE MOTA 853 118 -1.712 ANISOU 853 CG2 ILE 118 2077 2158 2792 -202 308 -530 ATOM 854 CG1 ILE 118 -2.877 37.031 52.368 1.000 24.69 ANISOU 854 CG1 ILE 118 4436 1808 3136 284 1382 - 414

- 118 -CD1 ILE 118 -3.786 37.025 53.582 1.000 29.63 855 ATOM ANISOU 855 CD1 ILE 118 6169 3096 1994 189 1258 - 1068 ATOM 856 ILE 118 -1.692 34.172 49.959 1.000 15.65 ANISOU 856 C ILE 118 2316 1549 2082 -89 573 - 117 MOTA 857 118 -0.463 34.035 49.802 1.000 14.59 0 ILE ANISOU 857 0 ILE 118 2240 1255 2051 16 286 2 1 4 MOTA 858 TRP 119 -2.523 33.139 49.784 1.000 14.44 N ANISOU 858 N_{i} TRP 119 2125 1592 1771 47 128 - 7 1 859 ATOM CATRP 119 -2.010 31.795 49.518 1.000 13.68 ANISOU 859 TRP CA119 1712 1529 1957 -61 220 4 0 119 -3.089 30.755 49.932 1.000 14.93 ATOM TRP 860 CЗ ANISOU 860 CВ TRP 119 1819 1729 2123 -234 295 - 35 119 -2.864 30.482 51.420 1.000 16.19 ATOM 861 CG TRP ANISOU 861 CG TRP 119 1640 2364 2146 -168 582 167 119 -2.116 29.430 51.993 1.000 20.41 ATOM 862 CD2 TRP ANISOU 862 119 3189 CD2 TRP 2414 2151 202 523 405 ATOM 863 CE2 TRP 119 -2.177 29.580 53.392 1.000 19.84 ANISOU 863 CE2 TRP 119 3536 1818 2184 -439 234 137 119 -1.390 28.357 51.456 1.000 23.94 ATOM 864 CE3 TRP ANISOU 864 CE3 TRP 119 5382 1647 2068 561 126 400 ATOM 865 CD1 TRP 119 -3.340 31.223 52.460 1.000 20.05 ANISOU 865 CD1 TRP 119 3207 2343 2069 -9 189 -139 ATOM 866 NE1 TRP 119 -2.938 30.689 53.649 1.000 20.32 ANISOU 866 NE1 TRP 119 2806 2726 2188 -96 -68 ATOM 867 CZ2 TRP 119 -1.547 28.714 54.281 1.000 22.12 ANISOU 867 CZ2 TRP 119 4071 2256 2078 -17 105 2 2 ATOM 868 CZ3 TRP 119 -0.761 27.490 52.332 1.000 21.52 ANISOU 868 CZ3 TRP 119 4214 2168 1794 311 -193 1 119 -0.847 27.674 53.715 1.000 24.34 -193 1 9 7 CH2 TRP ATOM 869 ANISOU 869 CH2 TRP 119 5349 2047 1850 329 148 183 870 C ATOM 119 -1.521 31.634 48.095 1.000 14.27 TRP ANISOU 870 C 119 2180 1259 1985 -187 334 -119 -0.569 30.865 47.855 1.000 14.73 TRP 1985 -187 334 -65 871 0 ATOM TRP ANISOU 871 O 119 1996 1653 1946 -67 362 101 120 -2.109 32.325 47.116 1.000 13.99 TRP ATOM 872 N THR ANISOU 872 N THR 120 2231 1237 1848 106 627 -137 120 -1.541 32.275 45.762 1.000 15.19 873 CA THR ATOM ANISOU 873 CA THR 120 1903 2093 1774 9 435 - 242 120 -2.492 32.983 44.787 1.000 16.41 ATOM 874 CB THR ANISOU 874 120 1934 2304 1995 -331 152 6 120 -3.738 32.297 44.766 1.000 18.53 CB THR 1995 -331 152 6 6 ATOM 875 OG1 THR ANISOU 875 OG1 THR 120 1891 2288 2863 -236 195 4 0 7 120 -1.974 32.906 43.358 1.000 18.02 ATOM 876 CG2 THR ANISOU 876 CG2 THR 120 2135 120 2135 2602 2108 324 322 3 120 -0.145 32.870 45.727 1.000 14.19 322 3 1 8 ATOM 877 С THR ANISOU 877 С 120 1868 2050 1475 87 285 -167 120 0.756 32.299 45.078 1.000 13.62 THR MOTA 878 0 THR ANISOU 878 O THR 120 1864 1692 1620 301 354 217 ATOM 879 N GLN121 0.114 33.962 46.429 1.000 14.55 ANISOU 879 N GLN121 1721 1672 2136 304 175 - 67CA GLN CA GLN ATOM 880 121 1.459 34.548 46.483 1.000 15.80 ANISOU 880 121 2067 1666 2271 -18 -119 3 6 2 ATOM 881 С GLN 121 2.465 33.642 47.176 1.000 13.73 GLN 121 2.405 GLN 121 1747 ANISOU 881 С 1665 1806 -30 18 1 1 4 ATOM 882 0 GLN121 3.603 33.452 46.685 1.000 15.36 ANISOU 882 0 GLN121 2063 1688 2084 48 360 - 44 CB GLN ATOM 883 121 1.315 35.918 47.154 1.000 18.85 ANISOU 883 CВ GLN 121 2537 1426 3200 -73 -5 3 5 6 MOTA 884 CG GLN121 2.639 36.558 47.543 1.000 18.88 ANISOU 884 CG ${ t GLN}$ 121 2507 1788 2878 599 -248 MOTA 885 CD GLN 121 3.468 36.936 46.337 1.000 20.70

- 119 -ANISOU 885 CD GLN 121 2584 2138 -373 -85 231 3142 886 OE1 GLN 121 2.935 37.088 45.224 1.000 22.47 ANISOU 886 OE1 GLN 121 2695 2822 3019 -245 0 121 37.101 46.522 1.000 25.22 887 NE2 GLN 121 4.779 NE2 GLN ANISOU 887 121 2426 3344 3811 127 -131 1 3 8 5 888 N ATOM TYR 122 2.081 33.054 48.299 1.000 12.26 ANISOU 888 TYR 122 1747 1514 1399 99 - 55 - 258 ATOM 889 CA TYR 122 2.896 32.102 49.050 1.000 13.18 ANISOU 889 CA TYR 122 1901 1643 1464 -20 -253 - 160 890 31.724 50.364 1.000 13.78 MOTA CВ 122 2.211 TYR ANISOU 890 CB TYR 1435 1756 116 48 - 28 30.808 51.282 1.000 14.22 122 2045 MOTA 891 CG TYR 122 2.994 ANISOU 891 CG TYR 122 1966 1681 1758 101 68 1 0 1 892 ATOM CD1 TYR 122 4.271 31.120 51.722 1.000 17.48 ANISOU 892 CD1 TYR 122 1788 1972 2882 149 -5 4 2 0 893 MOTA CE1 TYR 122 5.003 30.284 52.576 1.000 18.55 ANISOU 893 CE1 TYR 122 2131 2050 2868 102 -404 2 5 1 394 CD2 TYR MOTA 122 2.445 29.619 51.731 1.000 20.72 ANISOU 894 CD2 TYR 122 3308 1366 3197 -519 -1524 3 2 3 895 ATOM CE2 TYR 122 3.140 28.773 52.574 1.000 25.40 ANISOU 895 CE2 TYR 122 3772 1812 4067 -782 -2084 873 896 ATOM CZTYR 122 4.413 29.101 52.992 1.000 20.93 ANISOU 896 CZTYR 122 2985 1742 3224 -96 -1145 3 1 3 897 ATOM OH TYR 122 5.068 28.230 53.826 1.000 29.87 ANISOU 897 ОН TYR 122 4830 1998 4522 -680 -3078 621 MOTA 898 С TYR 122 3.218 30.876 48.209 1.000 12.33 ANISOU 898 С TYR 122 1833 1439 1412 89 -218 8 8 ATOM 899 122 4.395 122 1896 0 TYR 30.507 48.117 1.000 14.25 ANISOU 899 0 TYR 1861 1656 339 -242 2 1 6 ATOM 900 N PHE 123 2.224 30.269 47.573 1.000 11.28 ANISOU 900 N PHE 123 1950 1297 1041 6 -151 185 MOTA 901 CA PHE 123 2.482 29.151 46.665 1.000 12.08 ANISOU 901 CA PHE 123 1731 1219 1640 64 - 60 2 6 ATOM 902 CB28.719 46.024 1.000 13.86 PHE 123 1.139 ANISOU 902 CB 1550 PHE 123 2048 1666 -104 - 276 - 82ATOM 903 CG123 1.311 PHE 27.516 45.099 1.000 14.44 ANISOU 903 CG PHE 123 2173 1677 1637 -475 - 9 4 142 MOTA 904 CD1 PHE 123 1.281 26.234 45.614 1.000 13.64 ANISOU 904 CD1 PHE 123 1857 1563 1764 -42 -702 - 236ATOM 905 CD2 PHE 123 1.511 27.664 43.729 1.000 13.81 ANISOU 905 CD2 PHE 123 1450 2164 1634 -420 -295 - 248 MOTA 906 CE1 PHE 123 1.468 25.141 44.795 1.000 17.16 ANISOU 906 CE1 PHE 123 2282 1819 2418 130 -855 - 644 ATOM 907 CE2 PHE 123 1.715 26.559 42.916 1.000 18.31 ANISOU 907 CE2 PHE 123 2098 -2657 2201 -1053 172 -845 MOTA 908 CZPHE 123 1.706 25.295 43.445 1.000 16.71 ANISOU 908 CZPHE 123 1442 2382 2526 -36 -306 -1077 MOTA 909 С PHE 123 3.489 29.511 45.581 1.000 13.48 ANISOU 909 С PHE 123 2004 1472 1645 236 157 1 8 MOTA 910 0 PHE 123 4.424 28.768 45.242 1.000 13.07 ANISOU 910 O PHE 123 1591 1498 1876 42 - 78 - 172 911 N MOTA ASP 124 3.294 30.684 44.948 1.000 13.83 ANISOU 911 N ASP 124 1490 1575 2189 51 207 288 MOTA 912 CA ASP 124 4.207 31.036 43.861 1.000 13.75 ANISOU 912 CAASP 124 1505 1330 2389 458 398 344 913 CBASP 124 3.708 124 2650 32.352 43.242 1.000 18.95 ASP ANISOU 913 CB 1970 2580 -63 926 656 ATOM 914 CG ASP 124 4.470 32.708 41.989 1.000 27.54 ANISOU 914 CG ASP 124 5327 2099 3036 -123 939 880 OD1 ASP ATOM 915 124 4.541 31.904 41.023 1.000 37.04 ANISOU 915 OD1 ASP 124 6362 3225 4485 108 2616 - 331

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ATOM ANISOU ATOM	917 917 918 9919 9919 9919 9919 9919 991	OCCOONNCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	AGLN AGLN AGLN AGLN AGLN AGLN AGLN AGLN	124 124 124 125 125 125 125 125 125 125 125 125 125	1396 999 1.396 1.396 1.399 1.399 1.390	33.843 35.09 31.164 1721 30.163 31.77 121.863 31.62.77 31.62.77 31.62.77 31.62.77 31.62.77 31.62.77 31.62.77 31.62.49 41.68.24 51.70.29 34.80.19 34.80.19 34.80.19 34.80.19 34.80.19 34.80.19 37.19	4151 44.328 43.674 45.899 46.4999 46.346 46.346 46.346 47.35 47.491 46.494 46.494 46.494 46.494 46.494 46.494 47.35 48.33 47.499 47	-1539 234 8 5 1 1.000 14.49 327 485 4 8 2 1.000 14.52 289 497 3 0 7 1.000 14.03 353 398 4 1 4 1.000 16.40 194 178 2 2 6 1.000 14.69 232 -25 1 5 3 1.000 14.10 7 -205 -201 1.000 18.13 787 -81 4 6 1.000 23.51 883 -36 -2 2 5 1.000 29.33 -667 237 -187 1.000 32.99 -678 -1642 1 5 6 1.000 27.38 -276 -580 -2 4 6 1.000 38.55 449 -2476 -669 1.000 30.26 -369 -835 3 6 3 1.000 12.36 248 -63 -2 6 4 1.000 30.26 -369 -835 3 6 3 1.000 12.36 248 -63 -2 6 4 1.000 13.39 219 -355 -3 77 0.500 16.24 188 202 -1 9 2 0.500 18.83 68 233 -2 1 0 0.500 23.94 -604 -757 3 3 0.500 35.94 -578 -1567 -4 7 8 0.500 24.63 -881 -2407 4 6 2 0.500 18.28 -68 -176 -1 0 5 0.500 18.42 344 -159 1 0 6
ATOM ANISOU ATOM ANISOU ATOM ANISOU	937 937 938 939 940 941 942 943 944 944 945	NE2 CB CC CC CD CD CE1 NE2	AGLN BGLN BGLN BGLN BGLN BGLN BGLN BGLN B	126 126 126 126 126 126 126 126 126 127 127 127 127	4491 6.525 1695 6.604 2537 5.442 2227 5.605 3289 4.231	1118 27.417 1137 27.750 2257 27.237 2573	3751 48.018 2245 49.497 2153 50.319	-881 -2407 4 6 2 0.500 13.36 602 -114 - 255 0.500 18.28 -68 -176 - 105 0.500 18.42 344 -159 1 0 6 0.500 25.36 -100 -223 9 5 3 0.500 25.02 1004 -83 - 298 1.000 12.95 307 -372 - 366 1.000 11.66 182 -85 1 5 9 1.000 11.61 146 -168 - 1 0 1.000 11.21 -92 -40 1 9 2

- 121 -СВ ANISOU 946 TYR 127 1346 1655 1491 -13 82 4 7 ATOM 947 CG TYR 127 5.791 26.069 41.496 1.000 11.49 ANISOU 947 CG TYR 127 1278 1428 1660 -4 - 4 1 0MOTA 948 CD1 TYR 127 6.550 24.928 41.270 1.000 11.28 ANISOU 948 CD1 TYR 127 1030 1334 1921 -87 -10033949 CE1 TYR ATOM 127 6.406 24.153 40.115 1.000 11.47 ANISOU 949 CE1 TYR 127 1164 1167 2027 -51 -53 2 1 950 CD2 TYR ATOM 127 4.871 26.410 40.500 1.000 11.98 CD2 TYR ANISOU 950 127 1677 1093 1784 204 -219 - 100 CE2 TYR MOTA 951 127 4.715 25.655 39.357 1.000 11.37 ANISOU 951 CE2 TYR 127 1539 1118 1665 140 -68 - 73127 5.494 ATOM 952 CZTYR 24.508 39.163 1.000 11.02 ANISOU 952 CZTYR 127 1202 1226 1760 91 48 - 125 953 ATOM ОН TYR 127 5.379 23.720 38.030 1.000 11.57 ANISOU 953 OH TYR 127 1547 1138 1712 94 177 - 34 ATOM 954 C TYR 127 8.386 27.392 42.882 1.000 10.83 ANISOU 954 C TYR 127 1296 989 1830 230 -43 3 7 8 ATOM 955 0 TYR 127 9.185 26.605 42.375 1.000 10.86 ANISOU 955 0 TYR 127 1292 1232 1603 164 -237 - 4228.716 42.865 1.000 10.98 956 ATOM N THR 128 8.565 ANISOU 956 N THR 128 1554 976 1642 212 -9 5 5 7 957 ATOM CATHR 128 9.766 29.305 42.295 1.000 11.80 ANISOU 957 CATHR 128 1686 1125 1673 -47 -169 3 8 6 ATOM 958 СВ THR 128 9.605 30.849 42.378 1.000 12.66 ANISOU 958 CB THR 128 1873 1074 1864 -52 -233 5 2 1 ATOM 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74 ANISOU 959 OG1 THR 128 2223 1597 2542 124 -457 9 9 8 ATOM 960 CG2 THR 128 10.878 31.510 41.893 1.000 16.54 ANISOU 960 CG2 THR 128-1871 778 3635 262 655 1 3 8 ATOM 961 C THR 128 11.040 28.828 42.964 1.000 11.26 ANISOU 961 C THR 128 1562 980 1738 -71 -162 148 ATOM 962 0 THR 128 11.995 28.458 42.258 1.000 12.16 ANISOU 962 0 THR 128 1769 1092 1758 17 26 2 7 9 963 ATOM N ALA 129 11.083 28.802 44.300 1.000 10.39 ANISOU 963 Ν ALA 129 1183 1001 1763 70 -118 147 ATOM 964 CAALA 129 12.273 28.386 45.037 1.000 10.59 ANISOU 964 CAALA 129 1206 945 1873 -69 -170 281 ATOM 965 CB ALA129 12.113 28.603 46.536 1.000 12.46 CB ALA ANISOU 965 129 2113 851 1769 82 -218 577 MOTA 966 С ALA 129 12.575 26.906 44.802 1.000 11.35 ANISOU 966 С 129 1258 ALA 883 2170 -16 -141 410 ATOM 967 0 129 13.738 ALA 26.485 44.641 1.000 10.93 ANISOU 967 0 129 1202 ALA 1157 1796 -36 -213 1 26.086 44.750 1.000 12.27 -36 -213 1 2 1 ATOM 968 N SER 130 11.519 ANISOU 968 N SER 130 1280 984 2398 -65 -1 -24 ATOM 969 130 11.682 CA SER 24.650 44.512 1.000 10.89 ANISOU 969 CA130 1623 SER 876 1638 -85 44 3 7 0 ATOM 970 ASER 130 10.342 СВ 23.940 44.716 0.500 10.08 ANISOU 970 CB ASER 130 1432 603 1793 213 247 4 1 3 971 ATOM OG ASER 130 9.771 24.063 46.006 0.500 9.12 ANISOU 971 OG ASER 130 1021 651 1792 91 1 - 143 ATOM 972 CB BSER 130 10.364 23.919 44.765 0.500 10.60 ANISOU 972 CB BSER 130 1687 822 1521 -45 318 158 ATOM 973 OG BSER 130 9.418 24.098 43.734 0.500 16.22 ANISOU 973 OG BSER 130 1717 1289 3156 137 -525 3 4 8 ATOM 974 C 130 12.214 SER 24.373 43.110 1.000 10.53 ANISOU 974 С SER 130 1586 733 1684 -166 210 484 ATOM 975 0 SER 130 13.137 23.532 42.942 1.000 11.17 ANISOU 975 0 SER 130 1385 1012 1849 -151 -95 140 ATOM 976 Ν ARG 131 11.680 25.044 42.079 1.000 10.46 ANISOU 976 N ARG 131 1578 861 1534 -87 -65 9 9

- 122 -977 MOTA CA ARG 131 12.260 24.839 40.742 1.000 10.60 ANISOU 977 CAARG 131 1480 1110 1438 61 -288 978 ATOM CB ARG 131 11.426 25.553 39.679 1.000 12.99 ANISOU 978 CBARG 131 1893 1369 1673 63 -525 276 ATOM 979 CG ARG 131 10.003 25.065 39.431 1.000 13.64 ANISOU 979 CG ARG 131 1707 1735 1742 335 -559 - 86 ATOM 980 CDARG 131 9.349 25.669 38.206 1.000 17.71 ANISOU 980 CD 131 2078 ARG 1973 2677 81 - 983 701 ATOM 981 ΝE ARG 131 9.453 27.113 38.015 1.000 19.76 ANISOU 981 ΝE ARG 131 2716 2034 2757 -525 7 1 3 -25 ATOM 982 CZARG 131 8.629 28.004 38.568 1.000 21.24 ANISOU 982 CZARG 131 3688 1878 2503 -8 -128 647 MOTA 983 131 7.631 NH1 ARG 27.634 39.366 1.000 21.32 ANISOU 983 NH1 ARG 131 2792 3142 2166 -486 -667 5 7 984 ATOMNH2 ARG 131 8.771 29.310 38.361 1.000 27.83 ANISOU 984 131 4649 NH2 ARG 1822 4103 -90° -422 5 6 1 ATOM 985 С ARG 131 13.714 25.323 40.688 1.000 10.42 ANISOU 985 С ARG 131 1542 1078 1339 50 -103 1 ATOM 986 O. ARG 131 14.568 24.683 40.080 1.000 10.94 ANISOU 986 0 ARG 131 1544 1105 1506 177 -134 4 2 ATOM 987 N ALA 132 14.028 26.438 41.343 1.000 10.97 ANISOU 987 ALA 132 1477 N 1129 1563 74 - 364 - 45 ATOM 988 ALA 132 15.379 CA26.983 41.343 1.000 11.10 ANISOU 988 CA132 1539 ALA 944 1735 9 -102 ATOM 989 CB ALA 132 15.429 28.344 42.048 1.000 12.82 ANISOU 989 CB 132 1711 ALA 1171 1987 -48 -248 - 198ATOM 990 С 132 16.393 ALA 26.045 41.995 1.000 11.55 132 1085 1107 2197 -197 305 7 132 17.481 25.832 41.432 1.000 11.81 132 1081 1809 1599 -204 17 - 9 133 16.061 25.490 43.175 1.000 11.16 ANISOU 990 С ALA-197 305 745 MOTA 991 0 ALA ANISOU 991 0 ALA ATOM 992 N VAL ANISOU 992 N 133 1260 VAL 1356 1623 -148 51 3 5 0 MOTA 993 CAVAL 133 17.011 24.587 43.840 1.000 11.62 ANISOU 993 CAVAL 133 1505 1529 1380 -69 -297 8 9 ATOM 994 CB VAL 133 16.738 24.418 45.344 1.000 12.14 ANISOU 994 CB VAL 133 1376 1564 1674. -74 -25 364 ATOM 995 CG1 VAL 133 15.550 23.501 45.608 1.000 14.96 ANISOU 995 CG1 VAL 133 1705 2316 ATOM 996 CG2 VAL 133 17.981 ANISOU 996 CG2 VAL 133 1755 2340 1845 -341 -677 5 5 1 ATOM 997 C VAL 133 17.079 23.268 43.065 1.000 11.71 ANISOU 997 C VAL 133 1376 1363 1711 -24 -425 1 6 9 ATOM 998 0 VAL 133 18.198 22.733 42.925 1.000 11.55 ANISOU 998 0 VAL 133 1391 1453 1545 -4 -116 3 9 8 ATOM 999 Ν 134 15.982 22.758 42.480 1.000 12.87 ALA ANISOU 999 Ν ALA 134 1399 1973 1517 28 -334 -228 1000 CA MOTA ALA 134 16.084 21.557 41.621 1.000 10.57 ANISOU 1000 CA ALA 134 1106 1691 1220 153 -298 9 6 MOTA 1001 CB ALA134 14.699 21.096 41.186 1.000 12.20 ANISOU 1001 CB ALA 134 1254 1589 1794 35 - 303 - 127 ATOM 1002 C ALA 134 16.968 21.797 40.399 1.000 12.58 ANISOU 1002 C ALA 134 1393 1399 1987 272 -4 2 7 7 ATOM 1003 0 ALA134 17.712 20.924 39.970 1.000 11.01 ANISOU 1003 O ALA 134 1254 1358 1574 83 - 268 2 6 ATOM 135 16.908 22.995 1004 N ARG 39.809 1.000 12.03 ANISOU 1004 N ARG 135 1517 1230 1824 -62 -327 8 7 MOTA 1005 CA ARG 135 17.773 23.353 38.676 1.000 13.23 ANISOU 1005 CA ARG 135 1854 1158 2015 -270 -209 1 6 1 ATOM 1006 CB ARG 135 17.393 24.734 38.170 1.000 14.57 ANISOU 1006 CB ARG 135 2203 1339 1994 -45 -541 2 2 2 MOTA 1007 CG ARG 135 17.753 25.160 36.797 1.000 19.22

- 123 -ANISOU 1007 CG ARG 135 4204 1120 1980 -490 -433 150 1007 CG ARG 135 4204 1120 1980 -490 -433 1 1008 CD ARG 135 17.237 26.563 36.471 1.000 22.14 ANISOU 1008 CD ARG 135 4046 135 4046 1500 2868 -159 315 8 135 15.831 26.607 36.077 1.000 22.66 -159 315 822 1009 NE ARG ANISOU 1009 NE ARG 135 4239 1404 2965 -94 47 2 5 7 ARG 135 4239 1404 2965 -94 4725 ARG 135 14.802 27.184 36.684 1.000 21.69 1010 CZ ANISOU 1010 CZ ARG 135 4004 1906 2333 92 - 506 6 4 1011 NH1 ARG 135 14.917 27.843 37.833 1.000 22.26 ANISOU 1011 NH1 ARG 135 4114 2532 1812 460 -833 3 4 1 1012 NH2 ARG 135 13.582 27.113 36.149 1.000 22.31 ANISOU 1012 NH2 ARG 135 4000 2243 2234 -544 -419 8 1013 C ARG 135 19.251 23.275 39.057 1.000 12.70 MOTAANISOU 1013 C ARG 135 1742 1264 -119 -16 430 1821 1014 O ARG 135 20.069 22.818 38.238 1.000 14.67 ATOM ANISOU 1014 O ARG 135 2133 1529 1910 19 169 3 9 1 ATOM 1015 N GLU 136 19.572 23.712 40.266 1.000 12.15 ANISOU 1015 N GLU 136 1423 1372 1820 -36 70 43 ATOM 1016 CA GLU 136 20.960 23.630 40.763 1.000 14.52

ANISOU 1016 CA GLU 136 1622 1701 2194 -90 -197 3 7 1

ATOM 1017 CB GLU 136 21.212 24.513 41.981 1.000 15.59

ANISOU 1017 CB GLU 136 21.064 26.020 41.783 1.000 18.01

ANISOU 1018 CG GLU 136 21.064 26.020 41.783 1.000 18.01

ANISOU 1019 CD GLU 136 2010 1762 3071 -232 -153 1 2 6

ATOM 1019 CD GLU 136 21.798 26.484 40.537 1.000 20.18

ANISOU 1019 CD GLU 136 2071 2079 3519 -308 89 3 6 9

ATOM 1020 OE1 GLU 136 22.987 26.148 40.394 1.000 24.64

ANISOU 1020 OE1 GLU 136 21.195 27.150 39.670 1.000 24.19

ANISOU 1021 OE2 GLU 136 21.364 22.186 41.076 1.000 14.00

ANISOU 1022 C GLU 136 1338 1619 2361 -112 -442 2 2 3

ANISOU 1023 O GLU 136 22.508 21.781 40.833 1.000 13.86

ANISOU 1023 O GLU 136 1366 1890 2009 -100 -287 3 2 9

ANISOU 1024 N VAL 137 1309 1451 1715 1488 -2238 5 70 4 3 0 1016 CA GLU 136 20.960 23.630 40.763 1.000 14.52 ATOM ANISOU 1024 N VAL 137 1309 1451 1715 148 -223 8 5
ATOM 1025 CA VAL 137 20.753 19.896 41.771 1.000 12.49
ANISOU 1025 CA VAL 137 1369 1522 1853 240 -69 28 9
ATOM 1026 CB VAL 137 19.560 19.165 42.429 1.000 12.41 ANISOU 1026 CB VAL 137 1422 1424 1869 -67 -85 -204 ATOM 1027 CG1 VAL 137 19.728 17.634 42.401 1.000 12.55 ATOM 1027 CG1 VAL 137 19.728 17.634 42.401 1.000 12.55
ANISOU 1027 CG1 VAL 137 1371 1508 1892 182 185 1 1 1
ATOM 1028 CG2 VAL 137 19.355 19.607 43.852 1.000 11.35
ANISOU 1028 CG2 VAL 137 1461 1281 1572 182 -254 2 8 8
ATOM 1029 C VAL 137 1202 1428 2113 150 -16 8 5
ATOM 1030 O VAL 137 1202 1428 2113 150 -16 8 5
ATOM 1030 O VAL 137 1021 1683 2249 149 1 1 4 6
ATOM 1031 N LEU 138 20.309 19.562 39.401 1.000 10.28
ANISOU 1031 N LEU 138 1198 881 1829 -15 158 2 2 6
ATOM 1032 CA LEU 138 1312 1408 2024 110 273 -5 2
ATOM 1033 CB LEU 138 19.398 19.358 37.130 1.000 11.81
ANISOU 1033 CB LEU 138 19.398 19.358 37.130 1.000 11.81
ANISOU 1033 CB LEU 138 1260 1586 1642 -20 383 4 3
ATOM 1034 CG LEU 138 18.036 18.726 37.457 1.000 10.77
ANISOU 1034 CG LEU 138 1391 1397 1304 -83 219 2 1 3
ATOM 1035 CD1 LEU 138 1391 1397 1304 -83 219 2 1 3 1035 CD1 LEU 138 16.916 19.324 36.596 1.000 12.72 ANISOU 1035 CD1 LEU 138 1416 1587 1829 -59 -25 173 1036 CD2 LEU 138 18.052 17.207 37.320 1.000 14.32 ANISOU 1036 CD2 LEU 138 1986 1390 · 2065 -79 296 370 1037 C LEU 138 21.903 19.525 37.505 1.000 13.61 ANISOU 1037 C LEU 138 1305 2026 1840 -65

- 124 -LEU 138 22.695 18.760 36.920 1.000 14.97 ATOM 1038 0 ANISOU 1038 O LEU 138 1125 LEU 138 1125 2247 2313 105 234 17 ARG 139 22.184 20.816 37.614 1.000 13.26 234 178 1039 N ANISOU 1039 N ARG 139 1432 2046 1561 -155 219 317 1040 CA ARG 139 23.397 21.372 37.085 1.000 14.71 ANISOU 1040 CA ARG 1040 C 1041 C 139 1648 1941 2000 -27 502 447 139 24.636 20.815 37.775 1.000 15.16 ARG ANISOU 1041 C ARG 139 1425 2101 2235 -158 324 116 ATOM 1042 O ANISOU 1042 O ATOM 1043 CB ANISOU 1043 CB ARG 139 25.650 20.495 37.166 1.000 18.15 ARG 139 1628 2581 2688 18 612 3 3 9 ARG 139 23.394 22.926 37.206 1.000 19.67 ARG 139 1749 1923 3803 -196 186 252 ARG 139 24.418 23.487 36.237 1.000 28.66 1044 CG ATOM ANISOU 1044 CG ARG 139 3924 2584 4383 -2305 882 - 563 1045 CD ARG 139 24.245 24.997 36.111 1.000 39.58
ARG 139 6801 2389 5849 -3273 119 -1
ARG 139 24 910 25.660 37.210 1.000 47.91 ATOM ANISOU 1045 CD ATOM 1046 NE ATOM 1046 NE ARG 139 24 910 25.660 37.210 1.000 47.91 ANISOU 1046 NE ARG 139 9548 2435 6222 -2157 -1331 - ATOM 1047 CZ ARG 139 24.493 26.682 37.928 1.000 45.42 ANISOU 1047 CZ ARG 139 6941 4516 5802 -882 -2118 - ATOM 1048 NH1 ARG 139 23.316 27.273 37.722 1.000 64.33 ANISOU 1048 NH1 ARG 139 7248 8153 9039 93 -2965 -98 ATOM 1049 NH2 ARG 139 25.309 27.109 38.888 1.000 32.62 ANISOU 1049 NH2 ARG 139 5020 4758 2616 -2746 590 1 -2157 -1331 - 708 -882 -2118 -1238 ANISOU 1048 NH1 ARG 139 7248 8153 9039 93 -2965 -980 ATOM 1049 NH2 ARG 139 25.309 27.109 38.888 1.000 32.62 ANISOU 1049 NH2 ARG 139 5020 4758 2616 -2746 590 167 ATOM 1050 N ALA 140 24.562 20.684 39.096 1.000 14.85 ATOM 1051 CA ALA 140 1287 2204 2151 -517 -26 -46 ATOM 1051 CA ALA 140 25.730 20.257 39.856 1.000 15.80 ANISOU 1051 CA ALA 140 25.730 20.257 39.856 1.000 15.80 ANISOU 1051 CA ALA 140 25.444 20.442 41.330 1.000 19.36 ANISOU 1052 CB ALA 140 2685 2447 222 243 -435 -480 ANISOU 1053 C ALA 140 2685 2447 222 243 -435 -480 ANISOU 1053 C ALA 140 1555 2795 2054 12 -186 -458 ATOM 1053 C ALA 140 1555 2795 2054 12 -186 -458 ATOM 1054 O ALA 140 1555 2795 2054 12 -186 -458 ATOM 1055 N THR 141 1779 2532 2350 -528 218 -108 ATOM 1055 CA THR 141 1779 2532 2350 -528 218 -10 8 ATOM 1055 CA THR 141 1256 2401 2268 -192 -95 29 1 ATOM 1057 CB THR 141 1256 2401 2268 -192 -95 29 1 ATOM 1058 OG1 THR 141 1238 2200 2172 155 282 30 1 ANISOU 1058 OG1 THR 141 1238 2200 2172 155 282 30 1 ANISOU 1059 CG2 THR 141 1249 1565 1926 -31 295 47 6 ANISOU 1059 CG2 THR 141 1249 1565 1926 -31 295 47 6 ANISOU 1059 CG2 THR 141 1240 2077 2160 135 -47 17 7 ANISOU 1060 C THR 141 125.423 16.374 37.257 1.000 16.11 ANISOU 1060 C THR 141 125.423 16.374 37.257 1.000 16.11 ANISOU 1060 C THR 141 125.423 16.374 37.257 1.000 16.11 ANISOU 1060 C THR 141 125.423 16.374 37.257 1.000 16.11 ANISOU 1060 C THR 141 125.423 16.374 37.257 1.000 16.11 ANISOU 1060 C THR 141 125.423 16.374 37.257 1.000 16.11 ANISOU 1060 C THR 141 125.423 16.374 37.257 1.000 16.11 ANISOU 1060 C THR 141 125.423 16.374 37.257 1.000 16.11 ANISOU 1062 N GLY 142 25.474 17.416 36.446 1.000 17.75 ANISOU 1062 N GLY 142 25.474 17.416 36.446 1.000 17.75 ANISOU 1062 N GLY 142 25.474 17.416 36.446 1.000 17.75 ANISOU 1062 N GLY 142 25.611 17.263 34.987 1.000 17.32 93 - 2965 - 980
 142
 2127
 2197
 2416
 303
 260
 5

 142
 25.611
 17.263
 34.987
 1.000
 17.32
 ATOM 1063 CA GLY ANISOU 1063 CA GLY 142 1642 2494 2447 -160 453 517 ATOM 1064 C GLY ANISOU 1064 C GLY 142 24.426 16.556 34.358 1.000 16.37 142 1619 1893 2710 261 472 4 2 ATOM 1065 O GLY 142 24.654 15.824 33.379 1.000 18.43 ANISOU 1065 O ATOM 1066 N ${ t GLY}$ 142 2243 2558 2201 57 798 1 6 3 THR 143 23.232 16.738 34.907 1.000 13.99 ANISOU 1066 N THR 143 1531 1429 2356 83 430 3 5 0 ATOM 1067 CA THR 143 22.049 16.003 34.472 1.000 14.69 THR 143 1768 1591 2223 8 342 9 3 ANISOU 1067 CA ATOM 1068 CB THR 143 21.208 15.584 35.700 1.000 15.52

ANISOU 1068 CB THR 143 1457 1653 2785 55 419 5 2 9
ATOM 1069 OG1 THR 143 22.037 14.784 36.573 1.000 14.63
ANISOU 1069 OG1 THR 143 1296 1792 2471 52 434 3 6 9
ATOM 1070 CG2 THR 143 20.044 14.738 35.231 1.000 14.24
ANISOU 1070 CG2 THR 143 1761 1981 1669 3 379 1 9 2
ATOM 1071 C THR 143 21.135 16.785 33.532 1.000 13.96
ANISOU 1071 C THR 143 1553 1708 2044 128 479 -131
ATOM 1072 O THR 143 20.642 17.828 33.923 1.000 15.65
ANISOU 1072 O THR 143 2374 1580 1995 315 486 5 5
ATOM 1073 N GLU 144 20.928 16.279 32.322 1.000 15.65
ANISOU 1073 N GLU 144 1734 1904 2184 -156 260 -271
ANISOU 1074 CA GLU 144 18.917 16.693 31.362 1.000 17.30
ATOM 1075 C GLU 144 18.774 15.693 31.292 1.000 17.30
ANISOU 1075 C GLU 144 1686 2470 2417 -377 152 1 0 6
ANISOU 1075 C GLU 144 18.922 14.631 30.680 1.000 16.71
ANISOU 1076 O GLU 144 18.922 14.631 30.680 1.000 16.71
ATOM 1076 C GLU 144 18.922 14.631 30.680 1.000 16.71
ATOM 1077 CB GLU 144 19.568 17.063 28.825 1.000 37.93
ANISOU 1077 CB GLU 144 19.568 17.063 28.825 1.000 37.93
ANISOU 1079 CD GLU 144 19.568 17.063 28.825 1.000 37.93
ANISOU 1079 CD GLU 144 19.568 17.063 28.825 1.000 37.93
ANISOU 1079 CD GLU 144 19.293 18.507 2821 -43 610 5 8
ANISOU 1079 CD GLU 144 19.293 18.507 28.2466 1.000 43.55
ATOM 1079 CD GLU 144 19.293 18.507 28.4666 1.000 43.55
ANISOU 1079 CD GLU 144 19.293 18.507 28.4666 1.000 43.55
ANISOU 1079 CD GLU 144 19.602 19.365 29.326 1.000 51.81
ANISOU 1080 0E1 GLU 144 18.766 18.798 27.367 1.000 40.12
ANISOU 1081 0E2 GLU 144 18.766 18.798 27.367 1.000 40.12
ANISOU 1081 0E2 GLU 144 18.766 18.798 27.367 1.000 40.12
ANISOU 1081 0E2 GLU 144 18.766 18.798 27.367 1.000 40.12 - 125 --2057 -2082 1767 -2497 -2259 2129 ANISOU 1094 OD2 ASP 146 6913 5052 3214 16 0 -1182
ATOM 1095 C ASP 146 13.860 14.441 28.552 1.000 16.65
ANISOU 1095 C ASP 146 2461 1904 1961 -128 580 - 40
ANISOU 1096 O ASP 146 13.041 14.605 29.457 1.000 15.67
ANISOU 1096 O ASP 146 2110 1935 1908 -334 381 - 420
ANISOU 1097 N GLY 147 13.871 15.149 27.429 1.000 20.60 ANISOU 1097 N GLY 147 3484 2416 1927 -26 419 1 ATOM 1098 CA GLY 147 12.903 16.212 27.155 1.000 18.06 ANISOU 1098 CA GLY 147 2771 2451 1638 -382 98 9 3 1927 -26 419 129

- 126 -GLY 147 13.361 17.574 27.609 1.000 18.73 GLY 147 2836 2195 2085 -524 143 52 GLY 147 12.676 18.570 27.282 1.000 18.34 GLY 147 2865 2416 1687 -413 -72 38 ATOM 1099 C ANISOU 1099 C -524 143 527 1100 0 ANISOU 1100 O -413 -72 389
 148
 14.498
 17.634
 28.316
 1.000
 16.35

 148
 2936
 1506
 1772
 -157
 142
 8

 148
 15.116
 18.889
 28.747
 1.000
 15.34
 1101 N GLYANISOU 1101 N GLY-157 142 8 8 ATOM 1102 CA GLY 148 2723 1279 1829 55 450 - 26 148 14.768 19.339 30.144 1.000 12.97 ANISOU 1102 CA GLYMOTA 1103 C GLY ANISOU 1103 C GLY
 148 2231
 1416
 1280
 -93
 -62
 4

 148 13.769
 18.930
 30.771
 1.000
 13.79
 148 2231 -62 4 0 7 1104 0 ATOM GLY ANISOU 1104 O GLY 148 2301 1376 1561 -164 88 3 2 3 1105 N ATOM VAL 149 15.604 20.224 30.718 1.000 12.81 ANISOU 1105 N VAL 149 15.388 20.724 32.079 1.000 11.81 VAL 149 1333 1390 1765 54 -92 120 ATOM 1106 CA ANISOU 1106 CA ATOM 1107 CB VAL 149 16.594 21.636 32.480 1.000 11.97 ANISOU 1107 CB VAL 149 1136 1696 1717 -100 246 1 2 4 ANISOU 1108 CG1 VAL 149 16.358 22.336 33.802 1.000 15.26 ANISOU 1108 CG1 VAL 149 1941 1922 1936 -195 55 -223 ATOM 1109 CG2 VAL 149 17.868 20.794 32.538 1.000 17.21 ANISOU 1109 CG2 VAL 149 1231 2045 3265 45 102 -10 3 ANISOU 1110 C VAL 149 14.101 21.482 32.280 1.000 11.32 ANISOU 1110 C VAL 149 1186 1303 1813 -78 131 4 7 9 ANISOU 1111 O VAL 149 13.378 21.218 33.253 1.000 12.35 ATOM 1111 O VAL 149 1664 1423 1608 -71 229 1 6 7 ANISOU 1112 N GLU 150 13.752 22.463 31.460 1.000 11.96 ANISOU 1112 N GLU 150 13.752 23.286 31.815 1.000 10.90 ANISOU 1113 CA GLU 150 12.592 23.286 31.815 1.000 10.90 ANISOU 1114 CB GLU 150 12.592 23.286 31.815 1.000 17.60 ANISOU 1114 CB GLU 150 12.608 24.601 30.999 1.000 17.60 ANISOU 1115 CG GLU 150 12.608 24.601 30.999 1.000 17.86 ANISOU 1115 CG GLU 150 2530 1470 2687 181 -161 9 0 7 ANISOU 1115 CG GLU 150 13.811 25.488 31.314 1.000 17.86 ANISOU 1115 CG GLU 150 2744 797 3246 246 434 20 2 ANISOU 1116 CD GLU 150 13.956 25.929 32.738 1.000 19.47 ANISOU 1116 CD GLU 150 13.956 25.929 32.738 1.000 19.47 ANISOU 1116 CD GLU 150 13.956 25.929 32.738 1.000 19.47 ANISOU 1116 CD GLU 150 3018 1353 3027 -97 -84 66 62 VAL 149 16.594 21.636 32.480 1.000 11.97 ATOM 1107 CB 3027 -97 -84 662 1117 OE1 GLU 150 12.951 26.005 33.475 1.000 18.21 ATOM ANISOU 1117 OE1 GLU 150 3035 1512 2373 -178 -321 5 3 6 1118 OE2 GLU 150 15.109 26.237 33.122 1.000 22.59 MOTA ANISOU 1118 OE2 GLU 150 2993 1664 3927 -38 -150 2 8 4 150 11.277 22.533 31.705 1.000 12.22 ATOM . 1119 C GLU ANISOU 1119 C GLU 150 1429 1540 ATOM 1120 O GLU 150 1429 1540 1676 235 147 ATOM 1120 O GLU 150 10.341 22.757 32.530 1.000 13.44
ANISOU 1120 O GLU 150 1739 1474 1894 315 470 28
ATOM 1121 N ALA 151 11.118 21.625 30.742 1.000 11.88
ANISOU 1121 N ALA 151 1783 1255 1477 94 45 2 5 3
ATOM 1122 CA ALA 151 9.881 20.844 30.698 1.000 13.82
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ANISOU 1123 CB ALA 151 9.739 20.094 29.390 1.000 14.89
ANISOU 1124 C ALA 151 9.792 19.864 31.867 1.000 12.71 1676 235 147 - 5 1474 1894 315 470 288 -100 -413 3 9 6 ALA 151 1489 2318 1851 22 -269 - 3 5 ALA 151 9.792 19.864 31.867 1.000 12.71 22 - 269 - 35 ATOM 1124 C ALA 151 1448 ANISOU 1124 C 1463 1920 93 41 4 2 4 ALA 151 8.655 ATOM 1125 0 19.580 32.280 1.000 14.69 ANISOU 1125 O ALA 151 1535 2114 1932 -242 204 - 108ATOM 1126 N 152 10.925 19.401 32.410 1.000 11.73 PHE ANISOU 1126 N 152 1598 PHE 1259 1598 120 9 271 1127 CA PHE ATOM 152 10.890 18.554 33.602 1.000 10.61 ANISOU 1127 CA PHE 152 1444 1061 1526 -33 ATOM 1128 CB PHE 152 12.293 17.981 33.820 1.000 10.23 ANISOU 1128 CB PHE 152 1317 1132 1437 -144 207 410 ATOM 1129 CG PHE 152 12.517 17.187 35.095 1.000 10.36

- 127 -ANISOU 1129 CG PHE 152 1388 1149 1399 -34 147 276 1130 CD1 PHE 152 12.036 15.896 35.229 1.000 11.24 ANISOU 1130 CD1 PHE 152 1479 1047 1743 114 -103 5 6 6 152 13.229 17.701 36.154 1.000 11.21 152 1489 1449 1319 85 174 1 = 1 1131 CD2 PHE ANISOU 1131 CD2 PHE 85 174 1 5 1 ATOM 1132 CE1 PHE 152 12.252 15.163 36.380 1.000 10.80 ANISOU 1132 CE1 PHE 152 1400 1234 1467 249 -111 3 7 3 1133 CE2 PHE ATOM 152 13.431 16.992 37.341 1.000 11.82 ANISOU 1133 CE2 PHE 152 1709 1622 1160 -276 414 2 152 12.932 15.717 37.457 1.000 11.97 -276 414 250 1134 CZ MOTA PHE ANISOU 1134 CZ PHE 152 1651 1604 1293 -255 296 170 1135 C MOTA 152 10.430 19.292 34.858 1.000 12.24 PHE ANISOU 1135 C PHE 152 1754 1168 1730 -10 339 8 4 MOTA 1136 0 152 9.728 18.729 35.726 1.000 11.49 PHE ANISOU 1136 O PHE 152 1672 1142 1550 200 109 2 153 10.809 20.575 34.997 1.000 11.86 109 277 1137 N ATOM LEU 153 10.809 20.3.5 153 2030 1236 1240 -6 73 156 153 10.532 21.386 36.155 1.000 11.99 1229 1437 -165 307 8 5 ANISOU 1137 N LEU 1138 CA LEU ANISOU 1138 CA LEU 153 1890 153 11.654 22.420 36.353 1.000 12.81 1139 CB LEU ANISOU 1139 CB LEU 153 1691 1381 1794 -72 97 - 40153 13.059 21.910 36.592 1.000 12.87 1140 CG LEU ANISOU 1140 CG LEU: 153 1762 1645 1483 146 269 6 4 1141 CD1 LEU 153 14.027 23.081 36.611 1.000 15.99 ANISOU 1141 CD1 LEU 153 1609 2006 2462 -49 450 - 431 1142 CD2 LEU ATOM 153 13.185 21.158 37.914 1.000 19.37 ANISOU 1142 CD2 LEU 153 3091 2462 1806 809 275 5 4 0 ATOM 1143 C LEU 153 9.179 22.084 36.123 1.000 12.96 ANISOU 1143 C LEU 153 ⁻1728 1253 1943 -336 360 MOTA 1144 0 LEU 153 8.709 22.506 37.193 1.000 13.24 ANISOU 1144 O LEU 153 1617 1302 2109 -443 481 -182ATOM 1145 N ASP ANISOU 1145 N ASP ATOM 1146 CA ASP ANISOU 1146 CA ASP 154 8.568 22.203 34.955 1.000 13.29 154 1643 1457 1951 60 517 2 8 0 154 7.195 22.671 34.764 1.000 14.21 154 1862 1255 2280 313 631 683 1147 CB ATOM ASP 154 6.995 23.269 33.373 1.000 18.38 ANISOU 1147 CB ASP 154 2091 2156 2738 328 728 1475 1148 CG MOTA 154 5 . 534 23 . 367 32 . 929 1 . 000 22 . 95 ASP ANISOU 1148 CG 154 2323 3543 2855 676 430 1 154 4.685 23.607 33.820 1.000 20.85 ASP 430 1501 1149 OD1 ASP ATOM ANISOU 1149 OD1 ASP 154 2164 2368 3389 895 478 1 154 5.168 23.254 31.702 1.000 24.33 154 2989 3146 3110 228 48 112 154 6.294 21.455 34.985 1.000 11.22 478 1144 1150 OD2 ASP ANISOU 1150 OD2 ASP 48 1128 ATOM 1151 C ASP ANISOU 1151 C ASP 154 1594 1403 1265 123 147 4 20.729 34.015 1.000 13.31 147 410 ATOM 1152 0 ASP 154 6.043 ANISCU 1152 O ASP 154 2143 1728 1186 427 219 170 ATOM 1153 N 155 5.891 CYS 21.220 36.233 1.000 9.91 ANISOU 1153 N 1098 1243 -/o 19.881 36.627 1.000 9.41 1115 -13 154 1 CYS 155 1425 -76 186 2 7 MOTA 1154 CA CYS 155 5.446 ANISOU 1154 CA CYS 155 1294 -13 154 172 19.171 37.269 1.000 10.64 ATOM 1155 CB CYS 155 6.635 ANISOU 1155 CB CYS 155 1276 1015 1753 28 -51 -122 ATOM 1156 SG CYS 155 7.316 38.797 1.000 12.01 19.819 ANISOU 1156 SG CYS 155 1376 1554 1633 -195 -199 9 5 ATOM 1157 C 155 4.138 CYS 19.885 37.423 1.000 9.66 ANISOU 1157 C 155 1301 CYS 1355 1013 115 146 216 1158 0 MOTA 155 3.215 CYS 37.064 1.000 11.61 20.645 ANISOU 1158 O CYS 155 1349 1386 1676 130 116 294 1159 N ATOM 19.033 38.442 1.000 10.26 GLU 156 4.021 ANISOU 1159 N GLU 156 1263 1495 1139 -29 168 299

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ANISOU 1204 CB PHE 161 1594 1947 2851 384 58 6 4

ATOM 1205 CG PHE 161 -0.317 25.109 56.771 1.000 22.56

ANISOU 1205 CG PHE 161 -1.175 25.010 57.849 1.000 26.03

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ATOM 1207 CD2 PHE 161 0.822 25.901 56.885 1.000 25.34

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ANISOU 1250 O
               PRO
                    165 9948
                                7012
                                        3507
                                               -959 692 1750
ATOM
      1251 CB
                    165 -5.001 20.820 67.769 1.000 37.76
               PRO
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ANISOU 1251 CB PRO 165 3640 6479 4227 -1488 380 -717 ATOM 1252 CG PRO 165 -5.417 20.048 66.569 1.000 36.16 ANISOU 1252 CG PRO 165 3341 6449 3948 -518 -349 - 398 ATOM 1253 CD PRO 165 3440 6296 3828 -1656 -5 -604 ATOM 1254 N LEU 178 4.459 8.087 66.987 1.000 36.23 ANISOU 1254 N LEU 178 4.599 3338 5918 -26 1216 1175 ATOM 1255 CA LEU 178 4.994 9.117 66.116 1.000 28.63 ANISOU 1255 CA LEU 178 3397 3170 4312 377 1344 4 0 1 ATOM 1256 CB LEU 178 3497 3245 4688 760 752 -620 ATOM 1257 CG LEU 178 3497 3245 4688 760 752 -620 ATOM 1257 CG LEU 178 3557 2950 4674 667 371 -979 ATOM 1258 CD1 LEU 178 7.859 7.367 64.073 1.000 32.13 ANISOU 1259 CD2 LEU 178 3.885 9.909 45.420 1.000 27.18 ATOM 1259 CD2 LEU 178 3.885 9.909 65.420 1.000 27.18 ANISOU 1250 C LEU 178 3.885 9.909 65.420 1.000 27.18 ANISOU 1250 C LEU 178 3.885 9.909 65.420 1.000 39.60 ANISOU 1261 O LEU 178 2407 4624 8016 -1253 1290 218 3 ATOM 1261 O LEU 178 2407 4624 8016 -1253 1290 218 3 ANISOU 1261 O LEU 178 2407 4624 8016 -1253 1290 218 3 ANISOU 1261 O LEU 178 2407 4624 8016 -1253 1290 218 3 ANISOU 1262 N ARG 179 4.128 11.200 65.160 1.000 25.65 - 131 -356 -1656 -1154 ATOM 1262 N ARG 179 4.128 11.200 65.160 1.000 25.65 ANISOU 1262 N ARG 179 2220 3437 4089 -216 878 7 -216 878 741 ATOM 1263 CA ARG 179 3.231 11.973 64.321 1.000 25.04 ANTSOU 1264 C ARG 179 3.297 11.572 62.852 1.000 24.51 ANTSOU 1265 O ARG 179 2.558 2721 4434 39.99 - 8.9 ATOM 1265 O ARG 179 2.558 2721 4434 39.99 - 8.9 ATOM 1265 O ARG 179 2.55 3242 50.79 441 -332 - 25.6 ANTSOU 1266 CB ARG 179 3.517 13.480 64.451 1.000 28.58 ANTSOU 1266 CB ARG 179 3.980 31.7 3561 -110 -843.5 7 ATOM 1266 CB ARG 179 3.817 3.725 38.62 57 -957 -3.72 ATOM 1268 CD ARG 179 3.307 15.570 65.757 1.000 30.01 ANTSOU 1268 CD ARG 179 3.307 15.570 65.757 1.000 31.51 ANTSOU 1268 CD ARG 179 3.307 15.570 65.757 1.000 31.51 ANTSOU 1269 NE ARG 179 2.925 16.126 67.058 1.000 37.82 ANTSOU 1270 CZ ARG 179 2.897 17.425 67.292 1.000 39.43 ANTSOU 1271 NH1 ARG 179 3.213 18.286 66.331 1.000 59.73 ANTSOU 1271 NH1 ARG 179 3.213 18.286 66.331 1.000 59.73 ANTSOU 1271 NH1 ARG 179 1.745 4676 62.73 -1045 3177 1.72 2 ATOM 1273 N MET 180 2013 ARG 179 5661 3832 3094 275 -1463 -17.475 ATOM 1273 N MET 180 2013 ANTSOU 1273 N MET 180 2013 ANTSOU 1274 CA MET 180 4.655 10.539 61.108 1.000 20.07 ANTSOU 1275 C MET 180 2346 1965 3315 -349 -3001 51 ATOM 1275 C MET 180 2334 61.896 60.331 1.000 20.07 ANTSOU 1276 O MET 180 2337 ANTSOU 1277 CB MET 180 2337 ANTSOU 1277 CB MET 180 2337 ANTSOU 1277 CB MET 180 2571 ANTSOU 1279 CB MET 180 2936 ANTSOU 1280 CE MET 180 4.859 ANTSOU 1280 C ATOM 1263 CA ARG 179 3.231 11.973 64.321 1.000 25.04 ANISOU 1263 CA ARG 179 1860 3289 4365 69 641 1 5 275 -1463 -173 ANISOU 1280 CE MET 180 5917 3450 4690 -258 -2680 1204 ATOM 1281 N ALA 181 5.467 8.295 60.680 1.000 16.99 ANISOU 1281 N 181 2144 2139 2174 -90 -558 2 9 9 ALA

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ATOM 1282 CA ALA 181 6.396 7.168 60.676 1.000 16.12
ANISOU 1282 CA ALA 181 2275 1958 1890 -171 -3436 0 2
ATOM 1283 CB ALA 181 2275 1958 1890 -171 -3436 0 2
ATOM 1283 CB ALA 181 2857 2158 2673 -648 694 1 0 6
ANISOU 1281 CB ALA 181 7.576 7.409 59.738 1.000 15.43
ANISOU 1285 CB ALA 181 7.576 7.409 59.738 1.000 15.43
ANISOU 1285 CB ALA 181 7.576 7.409 59.738 1.000 15.43
ANISOU 1285 CB ALA 181 7.458 8.198 59.783 1.000 15.49
ANISOU 1286 CB ALA 181 7.458 8.198 59.783 1.000 15.49
ANISOU 1286 CB ALA 181 2263 1717 1925 -315 -3694 3 2
ATOM 1285 CB ALA 181 2268 1761 1858 -173 -2964 3 4
ATOM 1287 CD PRO 182 2517 1745 1829 32 -785 51 1
ANISOU 1287 CD PRO 182 2517 1745 1829 32 -785 51 1
ANISOU 1287 CD PRO 182 2321 2908 221 -210 -3061 124 0
ANISOU 1288 CA PRO 182 2321 2908 221 -210 -3061 124 0
ANISOU 1289 CB PRO 182 2573 1336 1706 -101 -866 29 9
ANISOU 1289 CB PRO 182 2577 1978 1600 16.02 0
ANISOU 1289 CB PRO 182 2570 1978 1607 170 -251 7 7
ATOM 1290 CC PRO 182 10.479 5.713 61.066 1.000 14.78 1
ATOM 1291 C PRO 182 2301 2071 1952 -199 -245 1001 1
ANISOU 1291 C PRO 182 2301 2071 1952 -199 -245 1001 1
ANISOU 1291 C PRO 182 2301 2071 1952 -199 -245 1001 1
ANISOU 1292 C PRO 182 2301 2071 1952 -199 -245 1001 1
ANISOU 1293 N HIS 183 9.569 7.460 56.730 1.000 14.90 A
ATOM 1293 N HIS 183 9.569 7.460 56.730 1.000 12.28 1
ATOM 1293 N HIS 183 9.589 7.460 56.730 1.000 12.28 1
ATOM 1294 CA HIS 183 1737 1312 1657 -467 -482 53 9
ANISOU 1295 CB HIS 183 1433 1495 1614 -254 435 15 6
ATOM 1295 CB HIS 183 1433 1495 1614 -254 435 15 6
ATOM 1295 CB HIS 183 1849 1969 1000 12.03 1.000 12.28 1400 12.99 CH HIS 183 1849 1969 1000 12.03 1.000 12.28 1400 12.99 CH HIS 183 1849 1969 1000 12.03 1.000 12.28 1400 12.99 CH HIS 183 1849 1969 1000 12.03 1.000 12.28 1400 12.99 CH HIS 183 1849 1969 1000 12.03 1.000 12.28 1400 12.99 CH HIS 183 1849 1969 1000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.000 12.03 1.0
           ANISOU 1308 CE1 TYR 184 1960 878 1964 173 -40 182
ATOM 1309 CD2 TYR 184 12.333 6.949 49.279 1.000 11.13
           ANISOU 1309 CD2 TYR 184 1252 1302 1674 109 -283 9 3
ATOM 1310 CE2 TYR 184 12.102 5.834 48.502 1.000 12.93
           ANISOU 1310 CE2 TYR 184 1944 1422 1546 49 -384 7 3

ATOM 1311 CZ TYR 184 11.898 4.611 49.121 1.000 13.14

ANISOU 1311 CZ TYR 184 1717 1304 1972 30 -611 6 7

ATOM 1312 OH TYR 184 11.663 3.490 48.343 1.000 15.45
            ANISOU 1310 CE2 TYR 184 1944
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- 133 -ANISOU 1312 OH TYR 184 2028 1471 2373 42 - 476 - 247 TYR 184 10.447 9.390 51.314 1.000 11.50 1313 C ANISOU 1313 C TYR 184 1445 1215 1709 -187 -201 3 4 8 TYR 184 9.362 8.797 51.089 1.000 11.75 ATOM 1314 0 ANISOU 1314 O TYR 184 1305 1308 1853 -106 -171 4 2 7 ATOM 1315 N ASP 185 10.784 10.557 50.743 1.000 10.79 ANISOU 1315 N ASP 185 1581 1069 1449 -141 -132 1 1 ASP 185 9.861 11.218 49.815 1.000 9.10 ASP 185 9.934 12.743 49.886 1.000 10.13 ASP 185 1427 1095 1327 -298 -178 1 1 ASP 185 9.540 13.388 51.185 1.000 11.79 ASP 185 1797 1350 1333 -250 -149 1 ASP 185 9.681 14.638 51.278 1.000 13.79 ASP 185 2050 1316 1875 135 -52 -12 ASP 185 9.114 12.755 52.189 1.000 13.31 ASP 185 1805 1848 1405 -411 -63 1 1 ASP 185 10.098 10.759 48.371 1.000 9.44 ASP 185 1036 1150 1401 -309 -26 1 1 ASP 185 11.234 10.469 48.005 1.000 10.64 ASP 185 11.234 10.469 48.005 1.000 10.64 ASP 185 1167 1376 1500 -127 -35 -2 ASP 185 1581 1069 1449 -141 -132 1 1 8 1316 CA ANISOU 1316 CA -326 23 2 0 6 1317 CB ANISOU 1317 CB -298 -178 1 7 7 1318 CG ANISOU 1318 CG -250 -149 1 1 1319 OD1 ASP ANISOU 1319 OD1 ASP -52 - 26 1320 OD2 ASP ANISOU 1320 OD2 ASP -411 -63 105 1321 C MOT.1 ANISOU 1321 C -309 -26 100 MOTA 1322 0 ANISOU 1322 O ASP -127 -35 -206 1323 N ATOM LEU ANISOU 1323 N LEU -272 -177 - 5 8 ATOM 1324 CA LEU ANISOU 1324 CA 186 1641 LEU 186 8.030 9.295 45.798 1.000 11.32 1325 CB LEU ANISOU 1325 CB 186 1652 929 1721 -111 17 -479 7.977 46.602 1.000 12.60 LEU 1326 CG LEU 186 7.989 ANISOU 1326 CG LEU 186 1408 1039 2340 -263 -200 - 166 1327 CD1 LEU 186 6.896 7.064 46.028 1.000 16.64 ANISOU 1327 CD1 LEU 186 1900 1373 3049 -634 -398 - 135 1328 CD2 LEU 186 9.356 7.332 46.629 1.000 13.84 ANISOU 1328 CD2 LEU 1245 186 1438 2575 -155 443 283 ATOM 1329 C 186 9.024 11.521 45.223 1.000 10.90 LEU ANISOU 1329 C LEU 186 1327 1211 1603 -3 -451 164 ATOM 1330 0 LEU 186 8.768 11.406 44.031 1.000 13.60 ANISOU 1330 O LEU 186 2067 1608 -211 -321 1 0 3 1494 SER 187 9.264 12.705 45.734 1.000 10.71 ATOM 1331 N ANISOU 1331 N SER 187 1546 1129 1393 -76 -282 3 1 8 1332 CA SER 187 9.401 13.943 44.998 1.000 10.49 ANISOU 1332 CA SER 187 1427 1191 1370 195 -107 4 8 8 SER 187 1427 1191 1370 195 -1074 15ER 187 9.221 15.103 46.002 1.000 10.56 SER 187 1105 1048 1857 298 161 5 SER 187 10.430 14.918 46.726 1.000 13.01 SER 187 1343 1432 2169 -132 -295 2 SER 187 10.774 14.062 44.336 1.000 10.47 SER 187 1447 862 1669 135 -3 145 SER 187 11.684 13.246 44.513 1.000 10.54 SER 187 1577 799 1629 183 -91 - 77 MET 188 10.962 15.095 43.502 1.000 9.78 ATOM 1333 CB ANISOU 1333 CB 161 532 ATOM 1334 OG ANISOU 1334 OG -132 -295 2 0 1 ATOM 1335 C ANISOU 1335 C ATOM 1336 0 ANISOU 1336 O 1337 N ATOM 188 10.962 15.095 43.502 1.000 9.78 MET 188 10.962 15.095 43.502 1.000 9.78
188 1419 978 1318 147 44 7 4
188 12.267 15.584 43.065 1.000 9.94
188 1394 942 1441 182 58 3 7
188 12.128 16.543 41.891 1.000 10.89
188 1523 840 1774 98 48 2 2 7
188 13.385 17.258 41.470 1.000 11.40
188 1403 1172 1756 46 -51 2 1 4
188 14.687 16.134 40.891 1.000 12.71
188 1619 1272 1940 139 137 1 ANISOU 1337 N MET 1338 CA MET ANISOU 1338 CA MET 1339 CB MET ANISOU 1339 CB MET 1340 CG MET ANISOU 1340 CG MET 1341 SD MET ANISOU 1341 SD 188 1619 MET 1272 1940 139 137 198 188 16.061 17.267 40.790 1.000 13.86 1342 CE MET ANISOU 1342 CE MET 188 1862 1399 2003 -2.911 - 9.0

- 134 -1343 C MET 188 12.946 16.217 44.291 1.000 12.13 ANISOU 1343 C MET 1344 0 MET ANISOU 1344 O MET 144 132 8 7 1345 N VAL ANISOU 1345 N 189 1290 1217 1292 53 -175 6 189 12.745 17.894 46.099 1.000 9.70 189 1290 VAL 1346 CA VAL VAL 189 1209 1057 1420 -212 -45 -VAL 189 13.618 19.154 45.979 1.000 9.97 ANISOU 1346 CA VAL -212 -45 -19 1347 CB 1347 CB VAL 189 1288 1103 1398 -238 129 1
1348 CG1 VAL 189 14.953 18.837 45.266 1.000 13.45
1348 CG1 VAL 189 1334 1410 2368 -236 390 1
1349 CG2 VAL 189 12.899 20.289 45.264 1.000 12.24 ANISOU 1347 CB VAL 189 1288 -238 129 189 ANISOU 1348 CG1 VAL 189 1334 -236 390 143 ANISOU 1349 CG2 VAL 189 1715 1349 CG2 VAL 189 1715 1242 1693 -25 150 2 1350 C VAL 189 11.469 18.245 46.871 1.000 10.10 150 295 ATOM 1351 O VAL 189 1089 1600 1149 -456 -156 ANISOU 1351 O VAL 189 10.405 18.399 46.250 1.000 9.53
ATOM 1352 N THR 190 11.609 18.327 48.187 1.000 8.66 ANISOU 1350 C VAL 189 1089 1600 1149 -456 -156 -VAL 189 10.405 18.399 46.250 1.000 9.53 -456 -156 - 73 -222 -1908 ATOM 1363 CD1 LEU 191 12.333 22.794 48.218 1.000 15.25

ATOM 1364 CD2 LEU 191 1685 2018 2091 -476 -214 -305

ATOM 1364 CD2 LEU 191 11.717 25.231 48.448 1.000 17.46

ANISOU 1364 CD2 LEU 191 2310 2044 2281 -14 17 60 4

ATOM 1365 C LEU 191 9.798 22.328 52.006 1.000 11.93

ANISOU 1366 O LEU 191 1275 1677 1579 56 -190 -372

ATOM 1366 O LEU 191 1275 1677 1579 56 -190 -372

ATOM 1366 O LEU 191 1276 2173 1676 1 -192 -601

ATOM 1367 N ILE 192 10.394 22.483 53.190 1.000 13.49

ANISOU 1367 N ILE 192 10.394 22.483 53.190 1.000 11.06

ANISOU 1368 CA ILE 192 9.671 22.539 54.443 1.000 11.13

ANISOU 1368 CA ILE 192 9.671 22.539 54.443 1.000 11.13

ANISOU 1369 CB ILE 192 9.927 21.304 55.330 1.000 12.94

ANISOU 1369 CB ILE 192 2099 1586 1232 -65 -9 -233

ANISOU 1370 CG2 ILE 192 2099 1586 1232 -65 -9 -233

ANISOU 1370 CG2 ILE 192 2479 1983 1641 -206 426 -215

ANISOU 1371 CG1 ILE 192 2633 1658 1601 -400 -48 -175 ANISOU 1371 CG1 ILE 192 2633 1658 1601 -400 -48 -1 ATOM 1372 CD1 ILE 192 9.845 18.765 55.339 1.000 25.71 ANISOU 1372 CD1 ILE 192 5869 1608 2290 -175 -1566 - ATOM 1373 C ILE 192 9.966 23.809 55.253 1.000 11.47 -400 -48 -175 -175 -1566 -301 - 135 -

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ANISOU 1402 CB PHE 201 7119 6892 4168 -1869 1937 -1899
ATOM 1403 CG PHE 201 10.130 18.113 71.545 1.000 46.41
ANISOU 1403 CG PHE 201 6643 6596 4396
                                        -2038 1879 -1497
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ATOM 1404 CD1 PHE 201 10.738 16.954 71.991 1.000 50.03 ANISOU 1404 CD1 PHE 201 7982 6634 4393 -2326 1092 -991 ATOM 1405 CD2 PHE 201 9.220 18.001 70.513 1.000 42.63 ANISOU 1405 CD2 PHE 201 5458 6427 4313 -1097 2449 -226 ATOM 1406 CE1 PHE 201 10.434 15.739 71.417 1.000 49.95 ANISOU 1406 CE1 PHE 201 8275 6464 4240 -2047 227 -716 ATOM 1407 CE2 PHE 201 8.901 16.783 69.934 1.000 41.38 ANISOU 1407 CE2 PHE 201 8.901 16.783 69.934 1.000 41.38 ANISOU 1408 CZ PHE 201 9.515 15.636 70.392 1.000 44.74 ANISOU 1408 CZ PHE 201 9.515 15.636 70.392 1.000 44.74 ANISOU 1408 CZ PHE 201 7075 6261 3663 -1063 1020 -975 ATOM 1409 C PHE 201 11.722 20.110 70.107 1.000 42.42 ATOM 1410 O PHE 201 11.722 20.110 70.107 1.000 47.79 ANISOU 1410 O PHE 201 11.007 20.941 69.536 1.000 47.79 ANISOU 1410 O PHE 201 11.007 20.941 69.536 1.000 47.79 ANISOU 1411 N VAL 202 12.477 19.232 69.449 1.000 34.04 ANISOU 1411 N VAL 202 12.477 19.232 69.449 1.000 34.04 ANISOU 1411 N VAL 202 4525 5852 2558 -1948 7 -425 ATOM 1412 CA VAL 202 12.535 19.245 67.93 1.000 25.09 ANISOU 1412 CA VAL 202 12.535 19.245 67.93 1.000 25.09 ANISOU 1412 CA VAL 202 3221 3752 2558 -1041 -182 9 9 ATOM 1413 CB VAL 202 13.988 19.286 67.489 1.000 22.88 - 136 --2326 1092 - 991 -1097 2449 -2268 -2047 227 -716 -578 2006 - 1844 -1063 1020 - 975 -1964 717 -1441 -762 691 -2416 ATOM 1413 CB VAL 202 3221 3752 2558 -1041 -182 9 ANISOU 1413 CB VAL 202 13.988 19.286 67.489 1.000 22.88 ATOM 1414 CG1 VAL 202 2832 3430 2432 -577

ANISOU 1434 C GLN 205 1412 1474 1338 49 -468 - 21
ATOM 1435 O GLN 205 13.707 12.927 60.606 1.000 13.97
ANISOU 1435 O GLN 205 1622 2235 1449 -293 -449 - 147
ATOM 1436 CB GLN 205 14.164 13.062 63.662 1.000 15.57
ANISOU 1436 CB GLN 205 2421 1925 1568 341 151 8 3
ATOM 1437 CG GLN 205 13.863 13.635 65.032 1.000 18.58
ANISOU 1437 CG GLN 205 3321 2286 1451 689 -129 8 2
ATOM 1438 CD GLN 205 3321 2286 1451 689 -129 8 2
ATOM 1438 CD GLN 205 3687 3465 2091 520 -499 -570
ATOM 1439 OE1 GLN 205 3687 3465 2091 520 -499 -570
ATOM 1439 OE1 GLN 205 3687 3464 4251 14 -270 -1800
ANISOU 1440 NE2 GLN 205 3350 3464 4251 14 -270 -1800
ANISOU 1440 NE2 GLN 205 3055 2465 3225 335 -592 -140
ATOM 1441 N ALA 206 15.893 13.401 60.893 1.000 12.63
ANISOU 1441 N ALA 206 15.893 13.401 60.893 1.000 12.63
ANISOU 1441 N ALA 206 15.893 13.401 60.893 1.000 12.63
ANISOU 1442 CA ALA 206 15.893 13.401 60.893 1.000 12.63
ANISOU 1442 CA ALA 206 15.893 13.519 58.528 1.000 16.34
ANISOU 1442 CA ALA 206 16.693 13.519 58.528 1.000 16.34
ANISOU 1444 C ALA 206 16.693 13.519 58.528 1.000 16.34
ANISOU 1444 C ALA 206 16.693 13.519 58.528 1.000 16.34
ANISOU 1444 C ALA 206 1489 2331 2230 -290 179 -341
ATOM 1444 C ALA 206 1489 2331 2230 -290 179 -341
ATOM 1445 O ALA 206 18.368 12.182 60.908 1.000 15.92
ATOM 1445 O ALA 206 18.368 12.182 60.908 1.000 15.86
ANISOU 1445 O ALA 206 18.77 1772 2377 150 -356 3 0
ATOM 1446 N GLU 207 17.707 10.712 59.305 1.000 16.98 - 137 --603 123 -277· ATOM 1445 O ALA 206 18.368 12.182 60.908 1.000 179 - 341 ANISOU 1446 N GLU 207 17.707 10.712 2377 150 - 356 3 0 ANISOU 1446 N GLU 207 1981 2086 2383 - 335 348 - 186 ANISOU 1447 CA GLU 207 1981 2086 2383 - 335 348 - 186 ANISOU 1447 CA GLU 207 1981 2086 2383 - 335 348 - 186 ANISOU 1447 CA GLU 207 20.082 10.688 3684 1.000 20.58 ANISOU 1448 C GLU 207 2198 1938 3684 1.000 18.75 ANISOU 1449 O GLU 207 18.938 10.953 57.503 1.000 18.75 ANISOU 1449 O GLU 207 18.948 10.953 57.503 1.000 18.23 ANISOU 1449 O GLU 207 18.665 8.612 58.676 1.000 25.81 ANISOU 1450 CB GLU 207 18.865 8.612 58.676 1.000 25.81 ANISOU 1451 CG GLU 207 19.879 7.737 58.429 1.000 30.08 ANISOU 1451 CG GLU 207 19.879 7.737 58.429 1.000 30.08 ANISOU 1452 CD GLU 207 19.494 6.356 57.959 1.000 29.93 ANISOU 1453 OEI GLU 207 19.491 6.356 57.959 1.000 29.93 ANISOU 1453 OEI GLU 207 19.491 5.471 ANISOU 1455 N VAL 208 21.146 10.997 ANISOU 1455 N VAL 208 21.146 10.997 ANISOU 1456 CA VAL 208 22.376 11.593 58.902 1.000 16.97 ANISOU 1455 N VAL 208 21.146 10.997 ANISOU 1456 CA VAL 208 22.376 11.593 58.902 1.000 16.36 ANISOU 1457 CB VAL 208 22.376 11.593 58.902 1.000 16.36 ANISOU 1458 CGI VAL 208 22.376 11.593 58.902 1.000 16.36 ANISOU 1458 CGI VAL 208 23.652 13.688 58.409 1.000 20.76 ANISOU 1458 CGI VAL 208 23.742 11.591 58.700 1.000 20.76 ANISOU 1458 CGI VAL 208 23.652 13.688 58.409 1.000 20.76 ANISOU 1458 CGI VAL 208 23.652 13.688 58.409 1.000 20.76 ANISOU 1458 CGI VAL 208 23.652 13.688 58.409 1.000 20.76 ANISOU 1458 CGI VAL 208 23.742 11.591 58.700 1.000 16.36 ANISOU 1459 CG2 VAL 208 23.752 13.815 58.720 1.000 16.36 ANISOU 1459 CG2 VAL 208 23.752 13.815 58.720 1.000 16.36 ANISOU 1459 CG2 VAL 208 23.752 13.815 58.720 1.000 16.36 ANISOU 1450 C VAL 208 23.752 13.815 58.720 1.000 16.36 ANISOU 1450 C VAL 208 23.752 13.815 58.720 1.000 20.76 ANISOU 1456 CN VAL 208 23.585 10.877 59.507 1.000 20.79 ANISOU 1456 CN VAL 208 23.585 10.877 59.507 11.000 20.74 ANISOU 1456 CN VAL 208 23.752 10.829 60.741 1.000 20.74 ANISOU 1456 CN VAL 208 23.752 10.829 60.741 1.000 20.74 ANISOU 1456 ANISOU 1461 O VAL 208 2436 2256 3187 460 206 544 ATOM 1462 N GLY 209 24.457 10.295 58.672 1.000 18.94 ATOM 1462 N GLY 209 24.457 10.295 58.672 1.000 16.34 ANISOU 1462 N GLY 209 1764 2445 2989 211 -494 1 1.000 16.34 ATOM 1463 CA GLY 209 25.558 9.508 59.194 1.000 24.01 ANISOU 1463 CA GLY 209 2171 3040 3910 549 -396 7 0.000 ATOM 1464 C GLY 209 25.123 8.364 60.082 1.000 25.00 ANISOU 1464 C GLY 209 2874 3156 3470 1406 772 6 4 211 -494 1 5 549 -396 7 0 9

1406 772 649

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ATOM	146		$\operatorname{GL} olimits_{Y} olimits_{GL} olimits_{Y} olimits_{GL} olimits_{Y} olimits_{GL} olimits_{Y} olimits_{GL} olimits_{Y} olimits_{Y} olimits_{GL} olimits_{Y} olimi$	209	9 25.850	7.934	60.991	1 000 7 5 0 0
ANISO			${ t GLY}$	209	9 4448	3946	5279	
\mathtt{ATOM}	146		GLY	210	23.951	7.786	59.869	
ANISO	U 146	6 N	GLY	210		2756		
ATOM	146	7 CA	GLY		23.477		3278	523 899 749
ANISO	U 146	7 CA	GLY	210) 4479	6.678	60.671	
ATOM	1468		GLY	210		2136	3427	1228 742 912
ANISO			GLY		5472	7.025	62.016	
ATOM	1469		GLY	210) 54/2	2099	3237	
ANISO			GLY	210	22.634	6.098	62.789	1.000 40.26
ATOM	1470			210	7322	2719	5256	1881 2759 2360
ANISOU			ALA	211	. 22.651	8.281	62.338	1.000 25.78
ATOM	1471		ALA	211	4671	2359	2763	1370 724 1197
ANISOU	1471 1471	CA	ALA	211	22.048	8.671	63.613	1.000 23.74
ANISOC			ALA	211	2966	3156	2896	727 339 663
	1472	CB	ALA	211	23.093	9.333	64.496	1.000 29.57
ANISOU			ALA	211	2957	4372	3906	834 96 6 9
ATOM	1473		ALA	211	20.900	9.626	63.360	1.000 21.19
ANISOU			ALA	211	3090	2611	2350	484 178 741
ATOM	1474		ALA	211	20.936	10.381	62.399	1.000 23.91
ANISOU			ALA	211	3771	2659	2653	
ATOM	1475	N	PHE	212	19.889	9.629	64.204	-30 -66 930 1.000 19.88
ANISOU			PHE	212	2603	2577	2375	
ATOM	1476	CA	PHE	212	18.814	10.613	64.130	
ANISOU	1476	CA	PHE	212	2581	2257	2432	1.000 19.13
ATOM	1477		PHE	212		12.006	64.489	284 -565 3 1 7
ANISOU			PHE	212	3004	2480	2115	1.000 20.00
\mathtt{ATOM}	1478	0	PHE	212	19.893	12.230		133 -640 6 8
ANISOU			PHE		2497	3558	65.569	1.000 21.10
ATOM	1479	CB	PHE	212	17.688	10.290	1964	-391 -406 2 2 2
ANISOU	1479	CB	PHE		2553	2616	65.096	1.000 21.37
ATOM	1480	CG	PHE	212	17.010	8.950	2952	293 -197 -184
ANISOU	1480	CG	PHE	212	2161	3496	64.912	1.000 23.45
ATOM	1481	CD1	PHE		16.369	8.377	3253	-376 -282 -558
ANISOU	1481	CD1	PHE	212	2545		65.990	1.000 23.33
\mathtt{ATOM}	1482	CD2	PHF	212	17.029	3115	3206	-382 -350 - 508
ANISOU	1482	CD2	PHF	212	2554	8.302	63.687	1.000 25.83
ATOM	1483	CE1	DHE	212	15.730	3962	3299	-622 -217 - 787
ANISOU	1483	CE1	DHE	212	3784	7.149	65.872	1.000 28.13
ATOM	1484	CE2	DHE			3544	3362	-1119 96 - 973
ANISOU	1484	CF2	DHE		16.419 2504	7.072	63.569	1.000 23 . 04
ATOM	1485	CZ	PHE	212	2504	2960	3289	382 -232 - 558
ANISOU	1485	C 7	PHE	212	15.781	6.486	64.651	1.000 27.88
ATOM	1486		THR		3658	3977	2957	-1072 -501 - 760
ANISOU	1486	VI IA	THR	213	19.076	12.936	63.578	1.000 18.30
ATOM	1487	C 2		213	2690	2083	2181	149 -583 - 93
ANISOU	1487	CA	THR	213	19.566	14.310	63.681	1.000 17.99
ATOM	1488		THR	213	1976	2139	2721	230 -686 - 287
ANISOU	1/20	CB	THR	213	20.515	14.586	62.498	1.000 20.43
ATOM	1489	001	THR	213	1798	2280	3683	140 -119 - 423
ANISOU	1400	061	THR	213	21.638	13.695	62.629	1.000 25.33
ATOM	1400	OGI	THR	213	2571	3378	3676	925 71 5 2 8
ANISOU	1490	CGZ		213	21.087	15.985	62.485	1.000 21.11
ATOM			THR	213	1935	2667	3420	-310 -289 - 747
	1491	<u></u>	THR	213	18.391	15.277	63.641	1.000 15.53
ANISOU			THR	213	1732	2135	2032	111 -557 - 167
ATOM	1492	0	THR	213	17.533	15.195	62.761	1.000 16.11
ANISOU			THR	213	1742	2197	2180	-327 -669 5 6
ATOM	1493	N	ASP	214	18.362	16.199	64.590	1.000 15.60
ANISOU			ASP	214	2025	2046	1857	
ATOM	1494	CA	ASP		17.380	17.256	64.672	64 -405 2 1.000 15.59
ANISOU	1494	CA	ASP	214	2130	1722	2072	2 -1010 - 242
ATOM	1495	CB	ASP	214	17.744	18.200		2 -1010 - 242 1.000 17.13
							55.022	±.000 ± / . ± 3

- 139 -ANISOU 1495 CB ASP 214 2528 1893 2086 -226 -1022 - ATOM 1496 CG ASP 214 17.612 17.672 67.219 1.000 20.21 ANISOU 1496 CG ASP 214 3138 2495 2045 -451 -1276 - ATOM 1497 OD1 ASP 214 17.079 16.571 67.460 1.000 20.87 ANISOU 1497 OD1 ASP 214 2778 2632 2518 -247 -505 150 ATOM 1498 OD2 ASP 214 18.076 18.401 68.127 1.000 28.05 1893 2086 -226 -1022 -247 -451 -1276 -148 -247 -505 1 5 1 214 5110 3118 2429 -257 -1997 214 17.314 18.146 63.441 1.000 15.14 214 2029 1822 1901 182 -574 -1 214 18.349 18.552 62.897 1.000 17.63 ANISOU 1498 OD2 ASP -257 -1997 -619 1499 C MOTA ASP ANISOU 1499 C ASP -574 - 319 1500 O ATOM 1500 O ASP 214 18.349 18.552 62.897 1.000 17.63

ANISOU 1500 O ASP 214 1956 2032 2710 -214 -810 - 1

ATOM 1501 N LEU 215 16.105 18.493 63.027 1.000 14.69

ANISOU 1501 N LEU 215 1936 1758 1887 38 -334 242

ATOM 1502 CA LEU 215 15.915 19.504 61.979 1.000 13.35

ANISOU 1502 CA LEU 215 1820 1753 1498 89 -22 5 9

ATOM 1503 CB LEU 215 15.352 18.819 60.734 1.000 14.24

ANISOU 1503 CB LEU 215 1735 2167 1506 -98 75 - 3

ATOM 1504 CG LEU 215 16.291 17.813 60.056 1.000 16.39

ANISOU 1504 CG LEU 215 2031 2285 1911 -340 320 -4

ATOM 1505 CD1 LEU 215 3139 2024 3427 -10 -801 -8

ATOM 1506 CD2 LEU 215 17.482 18.543 59.434 1.000 26.93

ANISOU 1506 CD2 LEU 215 1998 5409 2827 -1083 909 -5

ATOM 1507 C LEU 215 15.002 20.622 62.500 1.000 14.65

ANISOU 1507 C LEU 215 1770 1607 2190 86 -165 -95

ATOM 1508 O LEU 215 13.822 20.662 62.151 1.000 19.45 ASP MOTA -214 -810 - 15 -340 320 -424 -10 -801 -877 -1083909 - 542ATOM 1507 C LEU 215 15.002 20.622 62.500 1.000 14.65
ANISOU 1507 C LEU 215 1770 1607 2190 86 -165 - 9 5
ATOM 1508 O LEU 215 1748 2165 3476 116 -303 - 203
ATOM 1509 N PRO 216 15.552 21.523 63.314 1.000 15.99
ANISOU 1509 N PRO 216 2390 1970 1715 -164 21 - 175
ATOM 1510 CD PRO 216 16.955 21.601 63.757 1.000 19.37
ANISOU 1510 CD PRO 216 2900 2306 2155 -83 -790 - 548
ATOM 1511 CA PRO 216 14.760 22.620 63.846 1.000 18.68
ANISOU 1511 CA PRO 216 3104 2017 1976 12 -74 -420
ATOM 1512 CB PRO 216 3592 1517 1971
ATOM 1513 CG PRO 216 3592 1517 1971
ATOM 1513 CG PRO 216 3702 22.847 64.581 1.000 22.35
ANISOU 1513 CG PRO 216 17.030 22.847 64.581 1.000 22.35
ANISOU 1512 CB PRO 216 17.030 22.847 64.581 1.000 22.35
ANISOU 1514 C PRO 216 14.461 23.700 62.819 1.000 18.50
ANISOU 1515 O PRO 216 2752 2453 2325 -32 -375 1 9
ATOM 1516 N TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1516 N TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1517 CA TYR 217 3213 1981 2422 90 -482 -718
ATOM 1518 C TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1515 O PRO 216 2752 2453 2325 -32 -375 1 9
ATOM 1518 C TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1515 O PRO 216 2752 2453 2325 -32 -375 1 9
ATOM 1518 C TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1515 O TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1516 N TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1516 N TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1516 C TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1518 C TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1518 C TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1516 N TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1516 C TYR 217 14.347 26.647 62.283 1.000 23.92
ANISOU 1516 C TYR 217 14.39 26.314 62.768 1.000 30.46 6
ANISOU 1520 CB TYR 217 14.39 26.314 62.788 1.000 30.46 6
ANISOU 1520 CB TYR 217 18.891 3688 6615 -323 132 -11870
ATOM 1520 CB TYR 217 18.891 3688 6615 -323 132 -1945
ATOM 1520 CD TYR 217 10635 5155 6158 5100 5100 57.77 7
ANISOU 1523 CD2 TYR 217 1 ATOM 1522 CD1 TYR 217 11.853 28.763 63.285 1.000 54.26 ANISOU 1522 CD1 TYR 217 10311 3688 6615 -323 132 -1945 ATOM 1523 CD2 TYR 217 12.428 27.243 65.043 1.000 57.77 ANISOU 1523 CD2 TYR 217 10635 5155 6158 -1027 -1446 -193 ATOM 1524 CE1 TYR 217 12.011 29.816 64.174 1.000 60.33 ANISOU 1524 CE1 TYR 217 11807 4345 6772 -1101 -132 -2259 ATOM 1525 CE2 TYR 217 12.585 28.296 65.926 1.000 64.51 ANISOU 1525 CE2 TYR 217 12481 5199 6832 -1936 -1520 -207 -1027 -1446 -1931 -1936 -1520 -2074

ATOM 1526 CZ TYR 217 12 378 29.586 65.481 1.000 64.11 ANTSOU 1527 OH TYR 217 12047 30.39 65.481 1.000 64.11 ANTSOU 1527 OH TYR 217 12.536 30.39 65.388 1.000 63.69 ANTSOU 1527 OH TYR 217 112047 30.39 65.388 1.000 63.69 ATOM 1528 N ARG 218 14 418 27.374 61.188 1.000 24.08 ANTSOU 1528 N ARG 218 14 418 27.374 61.188 1.000 24.08 ANTSOU 1529 CA ARG 218 15.335 1611 3055 507 -1471 -145 ANTSOU 1529 CA ARG 218 15.335 1611 3055 507 -1471 -145 ANTSOU 1529 CA ARG 218 15.335 1611 3055 507 -1471 -145 ANTSOU 1530 CB ARG 218 16.326 2490 3245 -504 -1565 38 2 ATOM 1530 CB ARG 218 16.326 2490 3245 -504 -1565 38 2 ATOM 1531 CG ARG 218 16.326 2490 3245 -504 -1565 38 2 ATOM 1531 CG ARG 218 16.009 27.714 660.703 1.003 5.78 ANTSOU 1531 CG ARG 218 18.659 3087 4497 -1107 -733 -773 ANTSOU 1532 CD ARG 218 18.659 3087 4497 -1107 -733 -773 ANTSOU 1533 NE ARG 218 19.223 3264 4152 -1242 -244 -619 ANTSOU 1533 NE ARG 218 19.223 3264 4152 -1242 -244 -619 ANTSOU 1533 NE ARG 218 20.218 32.746 59.709 1.000 29.51 ANTSOU 1534 CZ ARG 218 20.218 32.746 59.709 1.000 29.51 ANTSOU 1535 NH1 ARG 218 20.883 3166 4170 60.452 -1075 ATOM 1536 NH2 ARG 218 20.218 32.646 59.709 1.000 27.44 ANTSOU 1536 NH2 ARG 218 20.218 31.665 60.464 1.000 33.18 ANTSOU 1536 NH2 ARG 218 20.218 32.674 59.709 1.000 27.44 ANTSOU 1536 NH2 ARG 218 20.583 31.665 60.464 1.000 31.05 ANTSOU 1537 C ARG 218 7353 1.046 4170 60.452 -1075 ATOM 1538 O ARG 218 14.514 29.533 59.295 1.000 27.44 9.000 37.400 37			_				- 140 -					
ATOM 1527 OH TYE 217 12 536 50.83 71.29 -1460 -817 -2160 0 ANISOU 1528 N ARG 218 14.418 5206 7153 -1832 -1191 -2064 ANISOU 1528 N ARG 218 14.418 5206 7153 -1832 -1191 -2064 ANISOU 1529 CA ARG 218 15.335 28.465 60.948 1.000 30.71 -145 ANISOU 1529 CA ARG 218 5932 2490 3245 -504 -1555 38 2 ATOM 1530 CB ARG 218 5932 2490 3245 -504 -1555 38 2 ANISOU 1530 CB ARG 218 5969 7797 447 -7100 35.08 82 ANISOU 1531 CG ARG 218 77.401 77.114 6 ANISOU 1531 CG ARG 218 16.326 27.775 60.526 -1397 -779 -3148 ANISOU 1532 CD ARG 218 19.223 87.775 60.526 -1397 -779 -3148 ANISOU 1533 NE ARG 218 19.223 87.775 60.526 -1397 -779 -3148 ANISOU 1533 NE ARG 218 19.223 87.745 59.709 1.000 29.51 8 ANISOU 1534 CZ ARG 218 20.218 28.620 32.413 59.424 19.224		152	6 CZ			7 12.378		65.481	1.00	0.64 1.1	ł	
ATOM 1528 N ARG 218 14.418 27.374 61.188 1.000 63.6 9 ATOM 1528 N ARG 218 14.418 27.374 61.188 1.000 24.08 ARG 218 15.335 28.465 60.948 1.000 24.08 ARG 218 15.335 28.465 60.948 1.000 30.7 1 145 ARG 218 15.335 28.465 60.948 1.000 30.7 1 14.5 ARG 218 15.335 28.465 60.948 1.000 30.7 1 14.5 ARG 218 15.335 28.465 60.948 1.000 30.7 1 14.5 ARG 218 15.335 28.465 60.948 1.000 30.7 1 14.5 ARG 218 15.335 28.465 60.948 1.000 30.7 1 14.5 ARG 218 15.335 28.465 60.948 1.000 35.707 3.4 ARG 218 15.335 28.455 60.948 1.000 35.707 3.4 ARG 218 15.335 28.455 60.948 1.000 35.707 3.4 ARG 218 15.335 28.455 60.948 1.000 35.707 3.4 ARG 218 15.345 22 38.746 60.073 3.7 3.7 7.3 ARISOU 1532 CD ARG 218 15.680 30.7 4.4 49.7 1.000 35.777 3.4 ARISOU 1533 NE ARG 218 19.223 28.746 50.526 1.000 34.46 61 9.4 ARISOU 1534 CZ ARG 218 20.218 28.620 58.830 1.000 33.18 40.00					. 21		2783	7129	-146	0 -817 -	2.1	6.0
ATOM 1528 N ARG 218 14.418 27.374 61.188 1.000 24.08 ATOM 1529 CA ARG 218 15.335 28.465 60.948 1.000 24.08 ATOM 1529 CA ARG 218 15.335 28.465 60.948 1.000 24.078 ATOM 1530 CB ARG 218 16.326 28.135 59.840 1.000 30.71 1.000 35.70 8 ATOM 1530 CB ARG 218 16.326 28.135 59.840 1.000 30.71 1.000 35.70 8 ATOM 1531 CG ARG 218 17.401 27.114 60.073 1.000 35.70 8 ATOM 1531 CG ARG 218 18.658 27.775 60.626 1.000 34.773 1.000 35.70 8 ATOM 1531 CG ARG 218 18.658 27.775 60.626 1.000 34.773 1.000 35.77 3 ATOM 1531 CG ARG 218 19.223 28.746 50.948 1.000 35.77 3 ATOM 1531 CG ARG 218 19.223 28.746 50.948 1.000 35.70 1.000 35.70 8 ATOM 1531 CG ARG 218 20.218 28.7465 29.77 9 32.6 7.785 28.790 1.000 35.73 1.000 35.73 1.000 35.70		U 152	7 OH					66.358	1.00	063.69	•	
ANTISOU 1528 N ARG 218 4482 1 51611 3055 507 -1471 -145 ANTISOU 1529 CA ARG 218 15.335 28.465 60.948 1.000 30.71 ANTISOU 1530 CB ARG 218 5932 2490 3245 -504 -1565 3 8 2 ANTISOU 1530 CB ARG 218 5969 2797 4662 -1397 -779 -3 4 8 ATOM 1531 CG ARG 218 18.658 3087 497 -1107 -733 -7 73 ANTISOU 1531 CG ARG 218 18.658 360 3087 497 -1107 -733 -7 73 ANTISOU 1533 NE ARG 218 18.658 3264 4152 -1242 -244 -6 1 9 ANTISOU 1533 NE ARG 218 4707 ARG 1133 NE ARG 218 4707 ARG 1133 NE ARG 218 820.839 ARG 218 1000 29.51 ANTISOU 1535 NH1 ARG 218 20.839 ARG 218 3087 ARG 218 3087 ARG 218 3087 ANTISOU 1535 NH1 ARG 218 20.839 ARG 218 3087	ATOM	152	8 N				5206	7153	-183	2 -1191	- 2	064
ANTSOU 1529 CA ARG 218 15-335		U 152	8 N						1.000	024.08	}	
ATOM 1530 CB ARG 218 5932 2490 3245 1-504 -1565 3 8 2 2 ANTSOU 1530 CB ARG 218 5969 ART 2737 59.840 1.000 35.08 ART 2738 497 -1107 -733 -773 4.000 4.000 1.000 29.51 ART 2738 ART		152	9 CA			3 15.335					- 1	4 5
ANTSOU 1530 CB ARG 218 16.326 28.135 59.840 1.000 35.08 ARG 218 5969 2797 4562 -1397 -779 -3 48 ANTSOU 1531 CG ARG 218 16.000 37.77 3 ANTSOU 1532 CD ARG 218 16.609 3087 466.027 1.000 35.77 ANTSOU 1533 NE ARG 218 18.658 27.775 60.626 1.000 34.46 ANTSOU 1533 NE ARG 218 19.223 28.746 59.709 1.000 29.51 ATOM 1534 CZ ARC 218 20.218 28.629 ANTSOU 1534 CZ ARC 218 20.218 28.6269 ANTSOU 1535 NH1 ARG 218 20.839 27.452 58.709 1.000 29.51 ANTSOU 1535 NH1 ARG 218 20.239 31.66 ATOM 1537 C ARG 218 14.511 ANISOU 1536 NE2 ARG 218 20.583 ANISOU 1537 C ARG 218 14.514 ANISOU 1539 N PRO 219 6290 ANTOM 1539 N PRO 219 6290 ANTOM 1539 N PRO 219 6290 ANTOM 1540 CD PRO 219 14.424 ANTOM 1540 CD PRO 219 14.424 ANTOM 1540 CD PRO 219 13.464 ANTOM 1541 CA PRO 219 13.464 ANTOM 1541 CA PRO 219 13.464 ANTOM 1542 CB PRO 219 13.464 ANTOM 1542 CB PRO 219 13.464 ANTOM 1544 C PRO 219 13.464 ANTOM 1545 C ARG 218 13.523 ANTOM 1546 C ARG 219 13.464 ANTOM 1540 CD PRO 219 13.300 ANTOM 1544 C PRO 219 13.300 ANTOM 1544 C PRO 219 13.300 ANTOM 1540 CD PRO 219 13.464 ANTOM 1540 CD PRO 219 13.300 ANTOM 1540 CD PRO 219 13.300					218	3 5932	2490					
ATOM 1531 CG ARG 218 17.401 27.114 60.073 1.000 35.77 ATOM 1532 CD ARG 218 18.650 37.775 60.626 1.000 35.77 ATOM 1533 NE ARG 218 18.650 37.775 60.626 1.000 34.46 61 9.000 31.000 31.18 ATOM 1534 CZ ARG 218 20.218 28.476 59.709 1.000 29.51 3.000 31.18 ATOM 1534 CZ ARG 218 20.218 28.476 59.709 1.000 29.51 3.000 31.18 ATOM 1535 NH1 ARG 218 20.218 28.476 59.709 1.000 29.51 3.000 31.18 ATOM 1535 NH1 ARG 218 20.839 31.66 4170 60.452 -10.75 2.000 31.18 ATOM 1535 NH1 ARG 218 20.839 31.66 4170 60.452 -10.75 2.000 31.18 ATOM 1535 NH1 ARG 218 20.839 31.66 4170 60.452 -10.75 2.000 31.18 ATOM 1535 NH1 ARG 218 20.839 31.66 4170 60.452 -10.75 2.000 31.18 ATOM 1535 NH1 ARG 218 20.839 31.66 4170 60.452 -10.75 2.000 31.18 ATOM 1535 NH1 ARG 218 20.839 31.66 4170 60.452 -10.75 2.000 31.18 ATOM 1536 NH2 ARG 218 14.513 29.655 60.464 1.000 31.0.5 3.73 -15.85 3.000 31.0 31.0 31.0 31.0 31.0 31.0 31.		153	0 CB		218	3 16.326	28.135	59.840	1 000	-1262	3 8	2
ANTSOU 1531 CG ARG 218 17.401 27.114 60.073 1.000 35.777 3 ARTOM 1532 CD ARG 218 18.658 27.775 60.626 1.000 34.46 ATOM 1533 NE ARG 218 19.223 28.746 59.709 1.000 29.51 ARG 218 20.218 20.218 27.452 58.709 1.000 29.51 ARG 218 20.218 20.218 20.218 20.218 20.218 20.218 20.218 20.218 20.218 20.218 20.218 20.218 20.218 20.218 20.224 27.452 58.709 1.000 29.51 20.200 27.44 ARTOM 1535 NH1 ARG 218 20.22 28.620 58.830 1.000 33.18 ARTOM 1536 NH2 ARG 218 20.239 27.452 58.709 1.000 27.44 ARTOM 1536 NH2 ARG 218 20.239 27.452 58.709 1.000 27.44 ARTOM 1537 C ARG 218 14.513 29.655 60.464 1.000 31.05 ARTOM 1538 O ARG 218 14.513 29.655 60.464 1.000 31.05 ARTOM 1539 N PRO 219 14.246 30.747 61.157 1.000 20.2.96 ARTOM 1539 N PRO 219 14.246 30.747 61.157 1.000 30.01 ARTOM 1540 CD PRO 219 14.246 30.747 61.157 1.000 30.01 ARTOM 1540 CD PRO 219 14.256 30.747 61.157 1.000 30.01 ARTOM 1540 CD PRO 219 13.464 ARTOM 1540 CD PRO 219 3472 ARTOM 1540 CD PRO 219 34		153	1 66			5969	2797	4562		7 3 3 . U 8 7 - 7 7 9 -	2 1	0
ANTSOU 1532 CD ARG 218 18.658 ANTSOU 1532 CD ARG 218 18.658 ANTSOU 1533 NE ARG 218 19.223 28.746 60.626 1.000 34.46 61 9 ANTSOU 1533 NE ARG 218 19.223 28.746 59.709 1.000 29.51 ATOM 1534 CZ ARG 218 20.218 28.620 58.830 1.000 33.18 ARG 218 4707 ANTSOU 1535 NH1 ARG 218 20.218 28.620 58.830 1.000 33.18 ARG 218 20.218 28.620 28.820 29.555 58.700 1.000 22.96 1.000 22.96 1.000 22.96 1.000 22.96 1.000 22.96 1.000 22.96 1.000 22.96 1.000 22.96 1.000 22.96 1.000 22.96 1.000 22.96 1.000 22.96 1.000 23.64 ARG 218 20.218 28.620 29.20		J 153	1 00		216	17.401		60.073	1.000	35.77	J 4	0
ANTSOU 1532 CD ARC 218 5680 326.4 4152 -1242-46 -6 19 ATOM 1533 NE ARG 218 4707 2579 3926 78 81 -629 ANISOU 1534 CZ ARG 218 20.218 326.4 4152 -1042-214 -6 19 ANISOU 1535 NH1 ARG 218 20.218 3166 4170 60 452 -1075 3926 78 81 -629 ANISOU 1535 NH1 ARG 218 20.28 39 7.452 316 4170 27.44 -8 19 1.000 27.4 4 ANISOU 1536 NH2 ARG 218 20.583 316 4170 60 452 -1075 3926 78 81 -629 3926 316 4170 60 452 -1075 3926 78 81 -629 3926 3926 3926 3926 3926 3926 3926 3		153	2 CD		218	8 6009			-1107	7 - 733 -	77	3
ANTSOU 1533 NE ARG 218 19.223 ANTSOU 1534 CZ ARG 218 20.218 ANTSOU 1535 NH1 ARG 218 20.218 ANTSOU 1535 NH1 ARG 218 20.218 ANTSOU 1535 NH1 ARG 218 20.2839 ANTSOU 1536 NH2 ARG 218 20.583 ANTSOU 1538 O ARG 218 14.513 ANTSOU 1538 O ARG 218 14.513 ANTSOU 1538 O ARG 218 14.513 ANTSOU 1538 O ARG 218 9873 ANTSOU 1539 N PRO 219 14.246 ANTSOU 1540 CD PRO 219 14.246 ANTSOU 1540 CD PRO 219 14.597 ANTSOU 1540 CD PRO 219 14.597 ANTSOU 1541 CA PRO 219 14.597 ANTSOU 1542 CB PRO 219 13.523 ANTSOU 1542 CB PRO 219 13.523 ANTSOU 1544 C PRO 219 13.523 ANTSOU 1544 C PRO 219 13.947 ANTSOU 1545 O PRO 219 13.523 ANTSOU 1545 O PRO 219 13.300 ANTSOU 1546 N ASP 220 15.269 ANTSOU 1547 CA ASP 220 3549 ANTSOU 1554 N ASP 220 15.269 ANTSOU 1554 C ASP 220 3706 ANTSOU 1555 OD 2 ASP 220 3706 ANTSOU 1554 N ALA 221 2748 ANTSOU 1555 NH1 ARG 218 20.21 25.684 ANTSOU 1555 OD 2 ASP 220 3714 ANTSOU 1555 OD 2 ASP 220 3706 ANTSOU 1555 OD 2 ASP 220 3714 ANTSOU 1555 OD 2 ASP 220 3714 ANTSOU 1555 OD 2 ASP 220 3706 ANTSOU 1554 N ALA 221 2748 ANTSOU 1555 NH1 ARG 218 20.22 21 25.684 ANTSOU 1554 N ALA 221 2748 ANTSOU 1555 NH1 ARG 218 20.22 21 25.684 ANTSOU 1554 N ALA 221 2748 ANTSOU 1556 CA ALA 221 2	ANISOU	J 153:	2 CD		218	, 10.038 : 5680			1.000	34.46		
ATOM 1534 CZ ARG 218 20.218 20.218 39.22		1533	3 NE		218	19.223	28 716	4152	-1242	-244 -	61	9
ANISOU 1534 CZ ARG 218 20.218 28.620 58.830 1.000 33.18 4170 60 452 -10.75		J 1533	NE		218	4707	2579	39.709		29.51		
ATOM 1535 NHI ARG 218 20.839 27.452 58.709 1.000 27.96 ANISOU 1535 NHI ARG 218 4202 2881 3341 -503 -373 -1585 ANISOU 1536 NH2 ARG 218 2327 3579 2817 233 -1117 -872 ANISOU 1537 C ARG 218 2327 3579 2817 233 -1117 -872 ANISOU 1538 O ARG 218 14.513 29.655 60.464 1.000 31.05 ATOM 1538 O ARG 218 14.114 29.533 59.295 1.000 40.40 ANISOU 1539 N PRO 219 14.246 30.747 61.157 1.000 30.017 ANISOU 1539 N PRO 219 14.246 30.747 61.157 1.000 30.017 ATOM 1539 N PRO 219 14.597 31.043 62.554 1.000 36.79 ANISOU 1540 CD PRO 219 13.464 31.841 60.549 1.000 36.79 ANISOU 1541 CA PRO 219 13.523 32.993 61.563 1.000 26.34 28.000 1543 CG PRO 219 13.947 32.372 62.825 1.000 32.44 ATOM 1543 CG PRO 219 13.947 32.372 62.825 1.000 32.44 ATOM 1544 C PRO 219 13.947 32.372 62.825 1.000 25.98 -340 0.000 1543 CG PRO 219 13.947 32.372 62.825 1.000 32.44 ATOM 1545 O PRO 219 13.947 32.372 62.825 1.000 25.98 -340 0.000 25.98 ANISOU 1542 CB PRO 219 13.947 32.372 62.825 1.000 32.44 ATOM 1546 N ASP 220 15.269 32.087 58.906 1.000 27.96 ANISOU 1546 CB PRO 219 13.300 32.995 58.412 1.000 36.17 ANISOU 1547 CA ASP 220 15.269 32.087 58.906 1.000 27.96 ANISOU 1546 CB ASP 220 3561 1.756 4506 57.705 1.000 27.96 ANISOU 1547 CA ASP 220 15.847 32.660 57.705 1.000 27.96 ANISOU 1548 CB ASP 220 3561 1.5697 31.434 558 1.000 32.09 ATOM 1540 CB ASP 220 3549 3142 4558 1.000 32.09 ATOM 1540 CB ASP 220 3706 32.79 31.434 558 1.000 27.96 ANISOU 1548 CB ASP 220 3706 32.79 31.434 558 1.000 27.96 ANISOU 1549 CG ASP 220 3706 32.79 31.434 558 1.000 29.61 3.79 3.79 3.79 3.79 3.79 3.79 3.79 3.79		1534	1 CZ		218	20.218	28.620	58.830	1 000	-629		
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ATOM 1538 O ARG 218 7353	ATOM	1537	' C	ARG	218	14.513			233	-1117	- 8 1	7 2
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ATOM 1540 CD PRO 219 14.597 ATOM 1541 CA PRO 219 13.464 ANISOU 1541 CA PRO 219 13.464 ANISOU 1542 CB PRO 219 13.523 ATOM 1543 CG PRO 219 13.523 ANISOU 1543 CG PRO 219 13.523 ANISOU 1543 CG PRO 219 13.947 ANISOU 1543 CG PRO 219 13.947 ANISOU 1544 C PRO 219 13.947 ATOM 1544 C PRO 219 13.947 ATOM 1545 O PRO 219 13.300 ANISOU 1545 O PRO 219 3472 ANISOU 1546 N ASP 220 15.269 ANISOU 1546 N ASP 220 15.269 ATOM 1547 CA ASP 220 15.847 ANISOU 1547 CA ASP 220 3549 ATOM 1548 CB ASP 220 3549 ATOM 1549 CG ASP 220 17.617 ANISOU 1549 CG ASP 220 17.697 ANISOU 1550 OD1 ASP 220 3714 ANISOU 1551 OD2 ASP 220 16.037 ANISOU 1551 OD2 ASP 220 16.037 ANISOU 1551 OD2 ASP 220 16.037 ANISOU 1555 CA ALA 221 2748 ANISOU 1555 CA ALA ALA ALA 221 15.840 ANISOU 1555 CA ALA 221 15.840 ANISOU 1555 CA ALA ALA 221 15.840 ANISOU 1555 CA ALA 221 15.840 ANISOU 1555 CA ALA ALA 221 15.840 ANISOU 1550 CA ALA 221 15.840 ANISOU 1550 CA ALA 2		1539	N		219			61.157	1.000	30.01		
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ATOM 1546 N ASP 220 15.269 32.087 58.906 1.000 25.98 4506 -389 -644 -815 1756 4506 -389 -644 -815 1756 4506 57.705 1.000 27.96 1.000 27.90		1545	0		219	13.300	32.950			30.61	. 0 :	,
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ATOM 1547 CA ASP 220 15.847 32.660 57.705 1.000 27.96 ATOM 1548 CB ASP 220 3951 1603 5071 -364 30 -8 2 4 ANISOU 1548 CB ASP 220 17.212 33.238 58.155 1.000 29.61 ATOM 1549 CG ASP 220 18.091 32.158 58.780 1.000 32.09 ATOM 1550 OD1 ASP 220 17.697 31.434 59.719 1.000 26.12 ATOM 1551 OD2 ASP 220 3714 32.088 58.281 1.000 29.09 ATOM 1551 OD2 ASP 220 16.037 31.726 56.525 1.000 29.09 ATOM 1552 C ASP 220 16.037 31.726 56.525 1.000 25.26 ATOM 1553 O ASP 220 16.641 32.095 55.515 1.000 28.28 ATOM 1554 N ALA 221 15.500 30.510 56.631 1.000 21.58 ATOM 1555 CA ALA 221 15.840 29.484 55.658 1.000 19.81 ATOM 1555 CA ALA 221 2986 1452 3090 -342 -224 - 3 15	ANISOU	1546	N	ASP	220	15.269	32.087			25.98		
ANISOU 1547 CA ASP 220 3951 1603 5071 -364 30 -824 ANISOU 1548 CB ASP 220 17.212 33.238 58.155 1.000 29.61 ATOM 1549 CG ASP 220 18.091 32.158 58.780 1.000 32.09 ATOM 1550 OD1 ASP 220 17.697 31.434 59.719 1.000 26.12 ANISOU 1550 OD1 ASP 220 19.241 32.088 58.281 1.000 29.09 ATOM 1551 OD2 ASP 220 19.241 32.088 58.281 1.000 29.09 ATOM 1552 C ASP 220 16.037 31.726 56.525 1.000 25.26 ATOM 1553 O ASP 220 16.641 32.095 55.515 1.000 28.28 ATOM 1554 N ALA 221 15.500 30.510 56.631 1.000 21.58 ATOM 1555 CA ALA 221 2748 ANISOU 1555 CA ALA 221 15.840 29.484 55.658 1.000 19.81 ATOM 1556 CB ALA 221 2786 1452 3090 -342 -224 -315	ATOM	1547	CA	ASP	220	15.847				-644 - 8	1 5	
ANISOU 1548 CB ASP 220 17.212 33.238 58.155 1.000 29.61 ATOM 1549 CG ASP 220 18.091 32.158 58.780 1.000 32.09 ATOM 1550 OD1 ASP 220 17.697 31.434 59.719 1.000 26.12 ATOM 1551 OD2 ASP 220 3013 3522 3390 -158 -289 - 9 7 ANISOU 1551 OD2 ASP 220 19.241 32.088 58.281 1.000 29.09 ATOM 1552 C ASP 220 16.037 31.726 56.525 1.000 25.26 ATOM 1553 O ASP 220 16.641 32.095 55.515 1.000 28.28 ATOM 1554 N ALA 221 15.500 30.510 56.631 1.000 21.58 ATOM 1555 CA ALA 221 2748 1770 3681 -288 178 -651 ANISOU 1555 CA ALA 221 15.840 29.484 55.658 1.000 19.81 ATOM 1556 CB ALA 221 178.60 30.510 56.658 1.000 19.81	ANISOU	. 1547	CA	ASP	220	3951		5071	1.000	27.96	4	
ATOM 1549 CG ASP 220 18.091 32.158 58.780 1.000 32.09 ATOM 1550 OD1 ASP 220 17.697 31.434 59.719 1.000 26.12 ATOM 1551 OD2 ASP 220 19.241 32.088 58.281 1.000 29.09 ATOM 1552 C ASP 220 16.037 31.726 56.525 1.000 29.09 ATOM 1553 O ASP 220 16.037 31.726 56.525 1.000 25.26 ATOM 1553 O ASP 220 16.641 32.095 55.515 1.000 28.28 ATOM 1554 N ALA 221 15.500 ANISOU 1554 N ALA 221 15.500 ANISOU 1555 CA ALA 221 2748 ANISOU 1555 CA ALA 221 2748 ANISOU 1555 CA ALA 221 2986 1452 3090 -342 -224 - 315					220	17.212	33.238	58.155	1 000	29 61	4	
ANISOU 1549 CG ASP 220 3706 3527 4961 625 978 6 1 5 ATOM 1550 OD1 ASP 220 17.697 31.434 59.719 1.000 26.12 ATOM 1551 OD2 ASP 220 19.241 32.088 58.281 1.000 29.09 ATOM 1552 C ASP 220 16.037 31.726 56.525 1.000 25.26 ATOM 1553 O ASP 220 16.641 32.095 55.515 1.000 28.28 ATOM 1554 N ALA 221 15.500 ANISOU 1554 N ALA 221 15.500 ANISOU 1555 CA ALA 221 2748 ANISOU 1555 CA ALA 221 2748 ANISOU 1555 CA ALA 221 2986 1452 3090 -342 -224 -315	ATOM				220	3549	3142	4558			, 6	
ATOM 1550 OD1 ASP 220 17.697 31.434 59.719 1.000 26.12 ATOM 1551 OD2 ASP 220 3013 3522 3390 -158 -289 - 9 7 ANISOU 1551 OD2 ASP 220 19.241 32.088 58.281 1.000 29.09 ATOM 1552 C ASP 220 16.037 31.726 56.525 1.000 25.26 ATOM 1553 O ASP 220 16.641 32.095 55.515 1.000 25.26 ATOM 1553 O ASP 220 16.641 32.095 55.515 1.000 28.28 ATOM 1554 N ALA 221 15.500 30.510 56.631 1.000 21.58 ATOM 1555 CA ALA 221 2748 1770 3681 -288 178 -651 ANISOU 1555 CA ALA 221 2986 1452 3090 -342 -224 -315		1549	CG		220	18.091				32.09	Ū	
ANISOU 1550 OD1 ASP 220 3013 3522 3390 -158 -289 - 9 7 ANISOU 1551 OD2 ASP 220 19.241 32.088 58.281 1.000 29.09 ATOM 1552 C ASP 220 3714 3756 3581 304 677 - 712 ANISOU 1552 C ASP 220 16.037 31.726 56.525 1.000 25.26 ATOM 1553 O ASP 220 16.641 32.095 55.515 1.000 28.28 ATOM 1554 N ALA 221 15.500 4088 1665 4994 -855 298 -434 ANISOU 1555 CA ALA 221 2748 1770 3681 -288 178 -651 ANISOU 1555 CA ALA 221 2748 1770 3681 -288 178 -651 ANISOU 1555 CA ALA 221 2986 1452 3090 -342 -224 -315	ATOM	1550	OD1	ASD	220	17 607	3527		625	978 61	. 5	
ATOM 1551 OD2 ASP 220 19.241 32.088 58.281 1.000 29.09 ATOM 1552 C ASP 220 16.037 31.726 56.525 1.000 25.26 ATOM 1553 O ASP 220 2508 1291 5800 354 1110 - 8 2 2 ANISOU 1553 O ASP 220 4088 1665 4994 -855 298 - 4 3 4 ANISOU 1554 N ALA 221 15.500 ANISOU 1555 CA ALA 221 2748 1770 3681 -288 178 - 6 5 1 ANISOU 1555 CA ALA 221 2986 1452 3090 -342 -224 - 3 1 5	ANISOU	1550	OD1	ASP	220	3013	31.434 3522	59.719	1.000	26.12	0.	
ATOM 1552 C ASP 220 16.037 31.726 56.525 1.000 25.26 ATOM 1553 O ASP 220 16.641 32.095 55.515 1.000 28.28 ATOM 1554 N ALA 221 15.500 30.510 56.631 1.000 21.58 ATOM 1555 CA ALA 221 15.840 29.484 55.658 1.000 19.81 ATOM 1556 CB ALA 221 2986 1452 3090 -342 -224 - 315	ATOM	1551	200	ACD	220	19.241				-289 - 9	7	
ANISOU 1552 C ASP 220 16.037 31.726 56.525 1.000 25.26 ATOM 1553 O ASP 220 16.641 32.095 55.515 1.000 28.28 ATOM 1554 N ALA 221 15.500 30.510 56.631 1.000 21.58 ATOM 1555 CA ALA 221 2748 1770 3681 -288 178 -651 ANISOU 1555 CA ALA 221 15.840 29.484 55.658 1.000 19.81 ATOM 1556 CB ALA 221 2786 1452 3090 -342 -224 -315	AMISOU	1551			220	3714			304	29.09 677 - 7	1 2	
ATOM 1553 O ASP 220 16.641 32.095 55.515 1.000 28.28 ANISOU 1553 O ASP 220 4088 1665 4994 -855 298 -434 ANISOU 1554 N ALA 221 15.500 30.510 56.631 1.000 21.58 ATOM 1555 CA ALA 221 2748 1770 3681 -288 178 -651 ANISOU 1555 CA ALA 221 2986 1452 3090 -342 -224 -315		1552			220	16.037				25 26	12	•
ANISOU 1553 O ASP 220 4088 1665 4994 -855 298 -434 ANISOU 1554 N ALA 221 15.500 30.510 56.631 1.000 21.58 ATOM 1555 CA ALA 221 2748 1770 3681 -288 178 -651 ANISOU 1555 CA ALA 221 15.840 29.484 55.658 1.000 19.81 ATOM 1556 CB ALA 221 2986 1452 3090 -342 -224 -315					220	2508		5800			2 2	
ATOM 1554 N ALA 221 15.500 30.510 56.631 1.000 21.58 ATOM 1555 CA ALA 221 2748 1770 3681 -288 178 -651 ANISOU 1555 CA ALA 221 15.840 29.484 55.658 1.000 19.81 ATOM 1556 CB ALA 221 2986 1452 3090 -342 -224 -315	ANISOU	1553			220	10.641	32.095		1.000	28.28		
ANISOU 1554 N ALA 221 2748 1770 3681 -288 178 -651 ANISOU 1555 CA ALA 221 15.840 29.484 55.658 1.000 19.81 ATOM 1556 CB ALA 221 2986 1452 3090 -342 -224 -315	ATOM	1554	N		221	15 500				298 - 4	3 4	
ANISOU 1555 CA ALA 221 15.840 29.484 55.658 1.000 19.81 ATOM 1556 CB ALA 221 2986 1452 3090 -342 -224 - 315		1554	N	ALA	221	2748		36.631				
ATOM 1556 CB ALA 221 2986 1452 3090 -342 -224 - 315		1555			221	15.840				1/8 - 6 19 07	5 1	
	ATOM	155 <i>c</i>			221	2986	1452				1 5	
			CD	why	221	17.130				19.51	1 3	

ANISOU 1556 CB ALA 221 2267 1497 3647 -648 45 -746 ATOM 1557 C ALA 221 14.718 28.469 55.489 1.000 17.71 ANISOU 1557 C ALA 221 13.866 28.356 56.380 1.000 20.97 ATOM 1558 O ALA 221 13.866 28.356 56.380 1.000 20.97 ANISOU 1559 N VAL 222 14.728 27.756 54.378 1.000 14.22 ANISOU 1559 N VAL 222 1560 1582 2262 -76 -92 -11 ATOM 1560 CA VAL 222 13.823 26.617 54.160 1.000 14.89 ANISOU 1560 CA VAL 222 13.823 26.617 54.160 1.000 14.89 ANISOU 1561 CB VAL 222 13.823 26.617 54.160 1.000 17.28 ANISOU 1561 CB VAL 222 13.079 26.779 52.830 1.000 17.28 ANISOU 1562 CG1 VAL 222 13.079 26.779 52.830 1.000 17.28 ATOM 1562 CG1 VAL 222 13.995 26.685 51.620 1.000 19.17 ANISOU 1563 CG2 VAL 222 1974 2625 2686 -446 -775 150 ATOM 1563 CG2 VAL 222 11.996 25.747 52.641 1.000 19.17 .36 ANISOU 1563 CG2 VAL 222 11.996 25.747 52.641 1.000 17.36 ANISOU 1565 CG2 VAL 222 11.996 25.747 52.641 1.000 17.36 ANISOU 1566 C VAL 222 11.996 25.747 52.641 1.000 17.36 ANISOU 1566 C VAL 222 11.996 25.747 52.641 1.000 17.36 ANISOU 1565 O VAL 222 11.996 25.747 52.641 1.000 17.36 ANISOU 1566 O VAL 222 11.996 25.339 54.263 1.000 12.66 ANISOU 1566 O VAL 222 11.980 1825 1881 104 -13 -199 ANISOU 1566 O VAL 222 15.828 25.320 53.893 1.000 12.66 ANISOU 1566 O VAL 222 15.828 25.320 53.893 1.000 12.98 ANISOU 1566 O VAL 222 15.828 25.320 53.893 1.000 12.98 ANISOU 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 14.681 22.956 54.749 1.000 10.70 ANISOU 1568 CB LEU 223 14.681 22.9552 54.749 1.000 10.70 ANISOU 1568 CB LEU 223 14.681 22.956 54.749 1.000 10.70 ANIS - 141 -ANISOU 1567 CA LEU 223 891 1704 1472 -26 -98 - 7 ATOM 1568 CB LEU 223 14.276 22.130 55.961 1.000 13.02 ANISOU 1568 CB LEU 223 1387 1968 1593 -419 289 --419 289 -108 ATOM 1569 CG LEU 223 14.739 20.683 56.106 1.000 17.41
ANISOU 1569 CG LEU 223 2434 2132 2050 -290 -476.5666
ATOM 1570 CD1 LEU 223 16.247 20.614 56.204 10.000 17.20
ANISOU 1571 CD2 LEU 223 13.983 20.076 57.282 1.000 33.63
ANISOU 1571 CD2 LEU 223 3981 4721 4077 -341 134 2949
ATOM 1572 C LEU 223 14.362 22.211 53.456 1.000 10.02
ANISOU 1573 C LEU 223 1000 1265 1543 58-319 8 8
ATOM 1573 C LEU 223 1000 1265 1543 58-319 8 8
ATOM 1574 N VAL 224 15.406 21.675 52.798 1.000 12.86
ANISOU 1574 N VAL 224 15.406 21.675 52.798 1.000 10.55
ANISOU 1575 CA VAL 224 15.227 20.932 51.553 1.000 11.98
ANISOU 1575 CA VAL 224 15.227 20.932 51.553 1.000 11.98
ANISOU 1576 CB VAL 224 15.227 20.932 51.553 1.000 11.98
ANISOU 1576 CB VAL 224 15.833 20.690 49.102 1.000 13.16
ANISOU 1577 CG1 VAL 224 15.833 20.690 49.102 1.000 13.16
ANISOU 1578 CG2 VAL 224 15.833 20.690 49.102 1.000 13.86
ANISOU 1578 CG2 VAL 224 15.837 22.941 50.156 1.000 12.57
ANISOU 1578 CG2 VAL 224 15.833 20.690 49.102 1.000 13.86
ANISOU 1578 CG2 VAL 224 15.833 20.690 49.102 1.000 13.86
ANISOU 1578 CG2 VAL 224 15.837 22.941 50.156 1.000 12.57
ANISOU 1578 CG2 VAL 224 15.837 22.941 50.156 1.000 12.57
ANISOU 1579 C VAL 224 15.837 22.941 50.156 1.000 12.57
ANISOU 1579 C VAL 224 15.837 22.941 50.156 1.000 12.57
ANISOU 1579 C VAL 224 15.837 22.941 50.156 1.000 13.86
ANISOU 1579 C VAL 224 15.837 22.941 50.156 1.000 13.86
ANISOU 1580 O VAL 224 15.837 12.94 50.156 1.000 13.86
ANISOU 1580 C VAL 224 15.85 18.553 51.533 1.533 31 24.84
ANISOU 1580 C PHE 225 14.585 18.553 51.533 1.533 35 22.679 -56
ATOM 1581 N PHE 225 14.585 18.553 51.533 1.533 1.534 1.000 11.38
ANISOU 1582 CA PHE 225 14.585 18.553 51.533 1.533 1.534 1.3000 11.34
ANISOU 1583 CB PHE 225 14.685 18.553 51.533 1.533 1.534 1.3000 11.34
ANISOU 1584 CG PHE 225 14.685 15.653 54.291 1.000 11.34
ANISOU 1584 CG PHE 225 14.685 15.653 54.291 1.000 15.28 ATOM 1569 CG LEU 223 14.739 20.683 56.106 1.000 17.41 ANISOU 1569 CG LEU 223 2434 2132 2050 -290 -476 5 ANISOU 1584 CG PHE 225 964 1369 1991 -251 -333 181 ATOM 1585 CD1 PHE 225 14.685 15.653 54.291 1.000 15.28 ANISOU 1585 CD1 PHE 225 1771 1777 2256 -98 -853 298 ATOM 1586 CD2 PHE 225 12.532 16.576 54.254 1.000 17.91 ANISOU 1586 CD2 PHE 225 1904 2748 2153 341 106 0

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- 142 -
                   1587 CE1 PHE 225 14.619 15.535 55.661 1.000 17.46
   ATOM
   ANISOU 1587 CE1 PHE 225 2449
   ANISOU 1587 CE1 PHE 225 2449 1862 2321 -249 -795 6 6
ANISOU 1588 CE2 PHE 225 12.447 16.474 55.612 1.000 19.35
                                                                                                                       -249 -795 6 6 6
   ANISOU 1588 CE2 PHE 225 2563
                                                                                 2678 2111
                                                  225 13.499 15.945 56.341 1.000 18.20
                                                                                                                      121 129 - 11
   ATOM 1589 CZ PHE
   ANISOU 1589 CZ PHE
                                                  225 2952
                                                  -501 -470 3 6
   ATOM 1590 C PHE
                                       PHE 225 1480 1285 1804 130 -201 4 2
PHE 225 14.019 17.160 49.163 1.000 12.77
PHE 225 1473 1466 1912 341 -118.3 8
CYS 226 15.940 16.032 49.521 1.000 9.62
   ANISOU 1590 C
                 1591 0
   ATOM
   ANISOU 1591 O
  ATOM 1592 N
ANISOU 1592 N
ATOM 1593 CA
ANISOU 1592 N CYS 226 954 1403 1296 -204 -407 2 9
ANISOU 1593 CA CYS 226 15.917 15.400 48.197 1.000 10.80
ATOM 1594 CB CYS 226 1432 1204 1468 -258 -310 - 5 9
ANISOU 1594 CB CYS 226 17.337 15.029 47.744 1.000 12.02
ATOM 1595 SG CYS 226 1539 1362 1666 -357 16 -1 2 5
ANISOU 1595 SG CYS 226 1627 1400 2192 -341 18 1 3 9
ANISOU 1596 C CYS 226 1627 1400 2192 -341 18 1 3 9
ANISOU 1596 C CYS 226 14.998 14.178 48.256 1.000 9.86
ANISOU 1597 O CYS 226 1190 1061 1495 -20 -293 - 1 6
ANISOU 1597 O CYS 226 1181 1280 1781 -129 -435 2 7 2
ANISOU 1598 N GLY 227 14.217 13.963 47.205 1.000 10.17
ATOM 1598 N GLY 227 1428 1010 1427 -258 -271 - 3 5
ANISOU 1599 CA GLY 227 13.370 12.806 47.053 1.000 9.73
ATOM 1599 CA GLY 227 13.908 11.769 46.074 1.000 9.48
ATOM 1600 C GLY 227 13.908 11.769 46.074 1.000 9.48
ANISOU 1600 C GLY 227 14.935 11.961 45.402 1.000 9.86
ANISOU 1601 O GLY 227 14.935 11.961 45.402 1.000 9.86
                                       CYS 226 954 1403 1296 -204 -407
ATOM 1601 O GLY 227 14.935 11.961 45.402 1.000 9.86 ANISOU 1601 O GLY 227 1321 1137 1290 -104 -179 7 8 ANISOU 1602 N ALA 228 13.217 10.631 45.971 1.000 9.17 ATOM 1603 CA ALA 228 1279 729 1477 109 -135 5 8 ANISOU 1603 CA ALA 228 13.650 9.529 45.108 1.000 9.41 ATOM 1604 CB ALA 228 13.15 887 1371 9 -74 -52 ANISOU 1604 CB ALA 228 12.727 8.296 45.256 1.000 10.50 ATOM 1605 C ALA 228 13.712 9.918 43.637 1.000 9.25 ATOM 1606 O ALA 228 1343 666 1507 -108 90 139 ANISOU 1606 O ALA 228 14.493 9.305 42.895 1.000 9.48 ATOM 1607 N ILE 229 12.970 10.907 43.143 1.000 10.30 ATOM 1608 CA ILE 229 13.074 11.311 41.727 1.000 10.87 ATOM 1608 CA ILE 229 13.074 ANISOU 1608 CA ILE 229 11.802 12.078 41.295 1.000 11.52
                                                                               1446 1487 -2 -159 251
                 1609 CB ILE 229 11.802 12.078 41.295 1.000 11.52
 ATOM
 ANISOU 1609 CB ILE 229 1257
                                                                               1473 1647
                                                                                                                   34 -57 3 6 2
 ATOM 1610 CG2 ILE 229 11.997 12.852 39.999 1.000 11.30 ANISOU 1610 CG2 ILE 229 1655 1211 1426 83 -189 15
ATOM 1611 CG1 ILE 229 1655 1211 1426 83 -189 156
ANISOU 1611 CG1 ILE 229 10.575 11.131 41.237 1.000 14.39
ATOM 1612 CD1 ILE 229 1031 2034 2402
                 1612 CD1 ILE 229 1031 2034 2402 -40 210 3
1612 CD1 ILE 229 10.676 10.093 40.138 1.000 19.20
                                                                                                                   -40 210 311
ANISOU 1612 CD1 ILE 229 2085 1723
                                                                                                 3489
                                                                                                                   -610 93 -138
                                      ILE 229 14.389 12.034 41.477 1.000 10.38
                 1613 C
 ATOM
 ANISOU 1613 C
                                      ILE 229 1293
                                                                               1405
                                                                                                 1247
                                                                                                                    -62 -169 3 2 2
                                      ILE 229 14.952 11.947 40.369 1.000 11.66
 ATOM
                 1614 0
 ANISOU 1614 O
                                      ILE 229 1805
ATOM 1615 N ALA 230 14.965 12.692 42.490 1.000 10.66

ANISOU 1615 N ALA 230 1476 1274 1300 -104 -151 3 5 6

ATOM 1616 CA ALA 230 16.312 13.259 42.338 1.000 11.21

ANISOU 1616 CA ALA 230 1473 975 1813 -57 -308 9 0

ATOM 1617 CB ALA 230 16.681 14.148 43.509 1.000 10.58
                                                                               1257
                                                                                                 1368
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- 143 -
ANISOU 1617 CB ALA 230 1350
                                  1295
                                          1375
                                                 62 - 106 126
                ALA 230 17.336 12.136 42.132 1.000 11.28
       1618 C
ATOM
ANISOU 1618 C
                ALA
                     230 1640 1037 1610 1 55 2 4 2
230 18.220 12.185 41.273 1.000 11.29
                      230 1640
ATOM
       1619 0
                ALA
ANISOU 1619 O
                ALA
                     230 1510 1240 1539 -189 -40 2
231 17.173 11.097 42.946 1.000 10.55
                     230 1510
                                                  -189 -40 288
       1620 N
ATOM
                 THR
ANISOU 1620 N
                 THR
                     231 1328
                                  894 1787 -262 -70 2 1 4
                     231 18.064 9.939 42.819 1.000 11.98
       1621 CA
                THR
ANISOU 1621 CA
                THR
                     231 1929
                                  1018
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                                                  0 -164 159
                                         43.878 1.000 10.76
                     231 17.717 8.865
       1622 CB
                THR
ANISOU 1622 CB
                THR
                     231 1381
                                  1070
                                           1636
                                                   -86
                                                       -453 2 4 6
       1623 OG1 THR
                     231 17.658 9.437
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ANISOU 1623 OG1 THR
                     231 1615
                                  1236
                                                   35 -115 277
                                           1641
                     231 18.765 7.752 43.880 1.000 12.57
       1624 CG2 THR
ATOM
ANISOU 1624 CG2 THR
                     231 1621 1314
                                         1840
                                                   160
                                                        -89 351
       1625 C
               THR
                     231 17.958 9.352 41.415 1.000 12.52
ATOM
               THR 231 1632 1500 1624 -145 42 1 1
THR 231 18.939 9.050 40.732 1.000 12.15
ANISOU 1625 C
       1626 0
ATOM
ANISOU 1626 O
               THR 231 1636 1233 1747
                                                  -17 86 2 2 4
ATOM
       1627 N
               LEU 232 16.717 9.154 40.959 1.000 11.14
       1627 N LEU 232 1608 1005 1620 90 -68 1 4 1 1628 CA LEU 232 16.446 8.522 39.675 1.000 12.47
ANISOU 1627 N
                LEU 232 1880 1203 1657
ANISOU 1628 CA
                                                  109 -169 4 5
       1629 CB
                     232 14.950 8.214 39.552 1.000 12.81
ATOM
                LEU
ANISOU 1629 CB
                LEU
                     232 1989 1225 1654
                                                  -78 -209 1 9
                     232 14.452 7.464 38.314 1.000 14.85
232 2171 1753 1719 -5 -410 -9 0
232 15.020 6.055 38.240 1.000 16.78
       1630 CG
ATOM
                LEU
ANISOU 1630 CG
                LEU
                                                -5 -410 - 96
       1631 CD1 LEU
ATOM
                     232 2693 1749 1932 72 -431 -487
232 12.914 7.411 38.291 1.000 15.70
232 2180 1866 1920 -278 -589 4 9 4
232 16.964 9.354 38.511 1.000 11.58
ANISOU 1631 CD1 LEU
       1632 CD2 LEU
ANISOU 1632 CD2 LEU
       1633 C
                LEU
               LEU 232 1452 1390 1559 309 -301 1 3 6

LEU 232 17.752 8.837 37.686 1.000 1 3.45

LEU 232 1808 1436 1867 320 -17 3 0

VAL 233 16.565 10.617 38.414 1.000 10.95
ANISOU 1633 C
ATOM
       1634 0
ANISOU 1634 O
ATOM
       1635 N
ANISOU 1635 N
                VAL 233 1428
                                  1210
                                           1522
                                                  -14 -210 0
       1636 CA VAL 233 16.948 11.421 37.242 1.000 11.70
ATOM
ANISOU 1636 CA
                VAL 233 1703 1345
                                                  975
                                           1397
       1637 CB
                VAL 233 16.156 12.743 37.215 1.000 11.14
ATOM
ANISOU 1637 CB VAL 233 1672 1272
                                           1287
                                                         276 7 3
                                                  -26
       1638 CG1 VAL 233 16.661 13.774 38.249 1.000 13.34
ATOM
ANISOU 1638 CG1 VAL 233 1834 1562
                                          1673 -205 653 -368
       1639 CG2 VAL 233 16.106 13.412 35.827 1.000 14.66
ATOM
ANISOU 1639 CG2 VAL 233 1992 1873
                                          1704 -4 -45 5 8 6
       1640 C
MOTA
                VAL 233 18.459 11.586 37.132 1.000 13.41
ANISOU 1640 C
                VAL 233 1712 1573
                                          1811
                                                   91 151 1 2 5
ATOM
       1641 0
                VAL 233 19.012 11.627 36.021 1.000 13.45
ANISOU 1641 O
                VAL 233 1844 1402
                                           1866
                                                   46 192 4 3 8
ATOM
       1642 N
                THR 234 19.188 11.665 38.250 1.000 13.13
ANISOU 1642 N
                THR 234 1457 1639
                                           1893
                                                   -139 223 126
MOTA
       1643 CA
                THR
                     234 20.613 11.930 38.244 1.000 13.00
ANISOU 1643 CA
                THR
                     234 1483 1600
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                                                   -183 428 143
ATOM
       1644 CB
                THR
                      234 21.069 12.726 39.465 1.000 12.46
ANISOU 1644 CB
                THR
                      234 1300
                                           1803
                                  1632
                                                         200 251
                                                   -32
MOTA
       1645 OG1 THR
                      234 20.825 11.941 40.639 1.000 13.71
ANISOU 1645 OG1 THR
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                                  1662
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                                                   192
                                                         202 291
       1646 CG2 THR
ATOM
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ANISOU 1646 CG2 THR
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                                  1565
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       1647 C
ATOM
                 THR
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ANISOU 1647 C
                 THR
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ATOM 1648 O	THR 234 22.659	10.710 38.233	1.000 15.81
ANISOU 1648 O ATOM 1649 N	THR 234 1546	2169 2293	61 27 2 1 7
ATOM 1649 N ANISOU 1649 N	GLY 235 20.767 GLY 235 1776	9.477 38.070	1.000 14.76
ATOM 1650 CA	GLY 235 1776 GLY 235 21.530	1576 2254 8.249 37.994	77 81 410
ANISOU 1650 CA	GLY 235 2053	8.249 37.994 1803 2486	1.000 16.69 304 35 189
ATOM 1651 C	GLY 235 22.243	7.862 39.275	304 35 1 8 9 1.000 16.83
ANISOU 1651 C ATOM 1652 O	GLY 235 1854	2031 2512	765 244 193
ATOM 1652 O ANISOU 1652 O	GLY 235 23.305 GLY 235 2074	7.237 39.194	1.000 19.67
ATOM 1653 N	GLY 236 21.665	2172 3225 8.227 40.425	1035 383 372
ANISOU 1653 N	GLY 236 1732	8.227 40.425 1327 2433	1.000 14.46 154 198 7 5
ATOM 1654 CA ANISOU 1654 CA	GLY 236 22.187	7.768 41.692	154 198 7 5 1.000 15.73
ANISOU 1654 CA ATOM 1655 C	GLY 236 2060 GLY 236 23.166	1381 2536	41 186 3 1 2
ANISOU 1655 C	GLY 236 23.166 GLY 236 1931	8.691 42.388 1332 2346	1.000 14.76
ATOM 1656 O	GLY 236 23.778	1332 2346 8.244 43.373	252 73 2 8 8
ANISOU 1656 O	GLY 236 1983	2197 2782	1.000 18.32 106 -105 8 4 4
ATOM 1657 N ANISOU 1657 N	GLN 237 23.318	9.938 41.953	1.000 13.99
ATOM 1658 CA	GLN 237 1831 GLN 237 24.209	1349 2137	158 165 170
ANISOU 1658 CA	GLN 237 1474	10.956 42.485 1304 2210	1.000 13.13
ATOM 1659 CB	GLN 237 24.629	11.948 41.383	367 -31 276 1.000 13.38
ANISOU 1659 CB ATOM 1660 CG	GLN 237 1367	1566 2151	99 72 1 5 9
ANISOU 1660 CG	GLN 237 25.390 GLN 237 1404	11.335 40.219 1529 2666	1.000 14.74
ATOM 1661 CD	GLN 237 25.816	1529 2666 12.428 39.257	518 410 3 3 3 1.000 17.22
ANISOU 1661 CD ATOM 1662 OE1	GLN 237 2039	2018 2486	-64 426 3 6 0
ATOM 1662 OE1 ANISOU 1662 OE1		13.208 39.522	1.000 20.60
ATOM 1663 NE2	GLN 237 1566 GLN 237 25.116	2334 3928 12.470 38.127	-10 -29 965
ANISOU 1663 NE2	GLN 237 2014	12.470 38.127 2093 2533	1.000 17.47 208 438 408
ATOM 1664 C ANISOU 1664 C	GLN 237 23.627	11.739 43.663	1.000 12.90
ATOM 1665 O	GLN 237 1474 GLN 237 24.332	1324 2104	72 -10 2 5 5
ANISOU 1665 O	GLN 237 1739	12.549 44.282 1888 2413	1.000 15.90 -291 74 - 84
ATOM 1666 N ANISOU 1666 N	VAL 238 22.365		-291 74 - 8 4 1.000 12.13
ANISOU 1666 N ATOM 1667 CA	VAL 238 1372 VAL 238 21.664	962 2276 212	-33 2 0 0
ANISOU 1667 CA	VAL 238 21.664 VAL 238 1169	12.182 45.082 1436 1920	1.000 11.91
ATOM 1668 CB	VAL 238 20.622		-121 -276 - 19 1.000 12.00
ANISOU 1668 CB ATOM 1669 CG1	VAL 238 1024	1179 2357	-6 199 - 3 1
ANISOU 1669 CG1	VAL 238 19.978 VAL 238 1530	13.999 45.601	1.000 13.07
ATOM 1670 CG2	VAT. 238 21 207	1668 1767 14.088 43.463	63 -232 - 222
ANISOU 1670 CG2	VAL 238 1795		1.000 14.00 -40 -2 181
ATOM 1671 C ANISOU 1671 C	VAL 238 20.990 VAL 238 1707	11.156 46.000	1.000 13.62
ATOM 1672 O	VAL 238 1707 VAL 238 20.252		-103 -40 - 22
ANISOU 1672 O	VAL 238 1702		1.000 12.64 -318 257
ATOM 1673 N ANISOU 1673 N	LYS 239 21.247	11.246 47.300	1.000 11.99
ATOM 1674 CA	LYS 239 1075 LYS 239 20.568	1404 2076	127 -101 7 4
ANISOU 1674 CA	LYS 239 20.568 LYS 239 1224		1.000 12.77
ATOM 1675 CB	LYS 239 21.382		-12 -124 8 6 1.000 12.23
ANISOU 1675 CB ATOM 1676 CG	LYS 239 1333	1155 2158	183 -234 - 28
ANISOU 1676 CG	LYS 239 20.953 LYS 239 1643	9.626 50.793	1.000 13.85
ATOM 1677 CD	LYS 239 21.927		187 -52 - 89 1.000 20.13
ANISOU 1677 CD ATOM 1678 CE	LYS 239 2893	1795 2961	10 -1185 5 8 8
10/8 CE	LYS 239 21.364		1.000 24.73

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ANISOU			LYS	239 4065	2250	3080	-348 -1466 1064
MOTA	1679		LYS	239 22.019	8.841	54.420	
ANISOU			LYS	239 5658	4315	2293	1610 -930 - 304
MOTA	1680		LYS	239 19.169	10.949	48.661	1.000 11.59
ANISOU			LYS	239 1207	1332	1866	-35 -82 6 4
ATOM	1681		LYS	239 18.976	12.191	48.708	1.000 12.32
ANISOU			LYS	239 1638	1294	1749	-2 -25 2 3 6
ATOM	1682		ALA	240 18.222	10.047	48.863	1.000 10.65
ANISOU			ALA	240 1248	1266	1534	-52 -185 - 88
ATOM	1683		ALA	240 16.884	10.368	49.354	
ANISOU			ALA	240 1292	1057	1531	-195 -37 -109
ATOM ANISOU	1684		ALA	240 15.784	9.782	48.466	1.000 13.46
ANISOU	1685		ALA	240 1195	2378	1543	-232 20 - 403
ANISOU			ALA ALA	240 16.784 240 1308	9.881	50.807	1.000 10.97
ATOM	1686		ALA	240 1308	1249 8.664	1611	-127 -142 4 9
ANISOU			ALA	240 2136	1242	51.059 1568	
ATOM	1687		PRC	241 16.967	10.783	51.782	-243 28 - 7
ANISOU			PRO	241 1723	1041	1466	1.000 11.13 160 -49 138
ATOM	1688	CD	PRO	241 17.172	12.237	51.654	1.000 11.17
ANISOU	1688	CD	PRO	241 1419	1204	1618	-180 -128 7 6
ATOM	1689		PRO	241 17.043	10.340	53.166	1.000 11.96
ANISOU			PRO	241 1597	1447	1499	-172 -32 193
ATOM	1690	CB	PRO	241 17.712	11.545	53.891	1.000 14.25
ANISOU			PRO	241 1875	1837	1701	-531 -383 2 4 2
ATOM	1691		PRO	241 17.286	12.724	53.069	1.000 13.61
ANISOU			PRO	241 2015	1446	1709	-596 -465 - 22
ATOM ANISOU	1692		PRO	241 15.708	10.072	53.861	
ATOM	1693		PRO PRO	241 1417	1610	1665	-175 -187 4 1 8
ANISOU			PRO	241 14.759 241 1359	10.829	53.655	1.000 12.28
ATOM	1694		ARG	242 15.700	1582 9.033	1723	-232 -468 8 1
ANISOU	1694	N	ARG	242 1775	1407	54.711 1664	1.000 12.75 -170 76 2 5 0
ATOM	1695		ARG	242 14.563	8.804	55.576	1.000 10.76
ANISOU	1695	CA	ARG	242 1292	1417	1380	-207 -281 2 1 1
MOTA	1696		ARG	242 14.614	7.405	56.223	1.000 15.02
ANISOU			ARG	242 2419	1368	1918	-357 117 294
ATOM	1697	CG	ARG	242 14.115	6.342	55.230	1.000 17.85
ANISOU			ARG	242 3373	1274	2135	9 -560 251
ATOM	1698		ARG	242 14.254	4.934	55.763	1.000 19.42
ANISOU			ARG	242 3148	1111	3120	506 503 116
ATOM ANISOU	1699	NE	ARG	242 15.667			1.000 20.71
ATOM	1700		ARG ARG	242 3225	2107	2538	938 638 212
ANISOU	1700	C 2	ARG	242 16.107 242 3198	3.444	56.416	1.000 23.22
ATOM	1701		ARG	242 3196	2206 2.567	3417 56.980	307 -544 5 8 9
ANISOU	1701	NH1	ARG	242 4097	2112	3083	1.000 24.46 307 387 195
ATOM	1702	NH2	ARG	242 17.416	3.184	56.438	1.000 25.41
ANISOU	1702	NH2	ARG	242 3402	2332	3921	819 -267 4 0 3
ATOM	1703	С	ARG	242 14.477	9.834	56.704	1.000 11.95
ANISOU			ARG	242 1571	1463	1506	-248 -214 1 0 7
ATOM	1704		ARG	242 15.469	10.377	57.213	1.000 13.65
ANISOU			ARG	242 1708	1439	2040	-322 -401 - 38
ATOM	1705		HIS	243 13.252	10.085	57.118	1.000 11.60
ANISOU			HIS	243 1657	1410	1342	-311 -206 5
ATOM ANISOU	1706	CA	HIS	243 12.942	11.056	58.158	1.000 11.49
ANISOU	1705		HIS	243 1855	1571	938 -30	
ANISOU	1707	C D	HIS	243 12.968	12.462	57.546	1.000 11.22
ATOM	1708		HIS HIS	243 1432	1379	1453	-231 -221 3 9
ANISOU	1708	ر <i>و</i>	HIS	243 12.133 243 1937	12.694	56.341	1.000 11.80
	1,00	CG	1173	243 1931	1171	1378	-31 -268 7 9

- 146 -1709 CD2 HIS 243 10.885 13.236 56.181 1.000 11.15 ANISOU 1709 CD2 HIS 243 1990 1106 1142 35 - 344 141 1710 ND1 HIS 243 12.538 12.345 55.086 1.000 12.29 ANISOU 1710 ND1 HIS 243 1670 1606 1395 -394 -91 8 1711 CE1 HIS 243 11.599 12.653 54.209 1.000 12.59 ANISOU 1711 CE1 HIS 243 1686 1740 1357 -522 -202 - 253 1712 NE2 HIS 243 10.585 13.204 54.841 1.000 10.77 ANISOU 1712 NE2 HIS 243 1612 1307 1172 -616 -268 - 36 1713 C HIS 243 11.605 10.737 58.812 1.000 12.49 ANISOU 1713 C HIS 243 1869 1570 1308 -321 -53 7 3 1714 0 HIS 243 10.807 9.949 58.271 1.000 12.26 ANISOU 1714 O HIS 243 1756 1404 1497 -188 -115 4 7 1715 N ATOM HIS 244 11.352 11.319 59.983 1.000 12.16 244 1464 1715 1442 -230 -112 -244 10.138 11.043 60.758 1.000 12.02 244 1606 1809 1152 -599 -167 -244 10.255 9.778 61.615 1.000 12.51 ANISOU 1715 N HIS -230 -112 - 32 1716 CA HIS MOTA ANISOU 1716 CA HIS -599 -167 - 24 1717 CB HIS ATOM ANISOU 1717 CB HIS 244 1655 1763 1334 -19 101 - 47 1718 CG 244 11.270 9.810 ATOM HIS 62.698 1.000 15.04 ANISOU 1718 CG HIS 244 2025 1723 1965 -178 -433 1 5 4 1719 CD2 HIS 244 11.276 10.380 63.923 1.000 18.19 ANISOU 1719 CD2 HIS 244 2946 2339 1627 36 - 732 297 1720 ND1 HIS 244 12.504 9.203 62.662 1.000 19.30 ANISOU 1720 ND1 HIS 2232 244 2303 2800 229 -708 2 6 6 1721 CE1 HIS 244 13.226 9.387 63.731 1.000 22.48 ANISOU 1721 CE1 HIS 244 2649 2734 3159 11 -1206 6 5 0 1722 NE2 HIS 244 12.476 10.120 64.531 1.000 22.33 ANISOU 1722 NE2 HIS 244 3088 2895 2500 -272 -1236 384 1723 C ATOM HIS 244 9.780 12.246 61.613 1.000 13.47 ANISOU 1723 C HIS 244 1897 1673 -362 254 6 7 1549 1724 0 ATOM HIS 244 10.603 13.165 61.798 1.000 13.48 ANISOU 1724 O HIS 244 1800 1726 1595 -283 139 -161 ATOM 1725 N ANISOU 1725 N VAL 245 8.551 12.245 62.130 1.000 15.26 VAL VAL 245 8.090 13.352 62.970 1.000 17.31

VAL 245 2108 2442 2026 -125 476 -161

VAL 245 6.939 14.169 62.360 1.000 17.33

VAL 245 6.551 15.334 63.286 1.000 25.25

VAL 245 2217 2966 4410 -137 1939 -1248

VAL 245 7.252 14.713 60.966 1.000 21.49

VAL 245 3070 2538 2556 -180 313 2 7 1

VAL 245 7.682 12.768 64.327 1.000 18.29

VAL 245 2123 2689 2137 -443 508 - 7 1

VAL 245 6.765 11.945 64.429 1.000 18.62

VAL 245 1810 2174 3089 -15 451 2 5 4

ALA 246 8.385 13.202 65.369 1.000 21.54

ALA 246 8.385 13.202 65.369 1.000 25.10

ALA 246 8.133 12.701 66.719 1.000 25.10

ALA 246 4596 2562 2379 94 -225 9 9 7

ALA 246 9.424 12.723 67.537 1.000 29.82 MOTA 1726 CA VAL ANISOU 1726 CA 1727 CB ATOM ANISOU 1727 CB 1728 CG1 VAL ATOM ANISOU 1728 CG1 VAL -137 1939 - 1248 ATOM 1729 CG2 VAL ANISOU 1729 CG2 VAL 1730 C ANISOU 1730 C 1731 0 ANISOU 1731 O ATOM 1732 N ANISOU 1732 N MOTA 1733 CA ANISOU 1733 CA ATOM 1734 CB ALA 246 9.424 12.723 67.537 1.000 29.82 ANISOU 1734 CB ALA 246 5381 3408 .2540 402 -889 1 3 2 5 ALA 246 7.080 13.545 67.412 1.000 31.20 ATOM 1735 C ANISOU 1735 C 4143 314 280 428 ALA 246 5079 2632 ATOM 1736 0 ALA 246 6.876 14.714 67.052 1.000 32.39 ANISOU 1736 O ALA 246 4706 567 3748 3853 1247 - 6 6 1737 N ATOM ALA 247 6.429 12.973 68.413 1.000 37.30 ANISOU 1737 N ALA 247 5548 5498 3126 92 640 8 3 5 ATOM 1738 CA ALA 247 5.585 13.794 69.271 1.000 40.42 ANISOU 1738 CA ALA 247 5434 6048 3878 15 1313 8 5 0 1739 C ALA 247 6.289 14.132 70.578 1.000 42.17

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ANISOU 1739 C
                                        ALA 247 6495
                                                                                   5891
                                                                                                       3636
                                                                                                                        -823 1720 3 4 1
                   1740 O ALA 247 7.048 13.338 71.136 1.000 41.63
1740 O ALA 247 5811 6371 3637 -1631 804 4
1741 CB ALA 247 4.280 13.067 69.525 1.000 47.17
  ATOM
  ANISOU 1740 O
                                                                                                                        -1631 804 425
  ATOM
  ANISOU 1741 CB ALA 247 5186
                                                                                 9059
                                          ALA 247 5186 9059 3676 -520 523 2683
SER 257 1.781 21.848 70.382 1.000 31.02
                                                                                                     3676
                    1742 N
  MOTA
  ANISOU 1742 N
                                          SER
                                                    257 4109
                                                                                 5558 2119
                                                                                                                         137 -235 -810
  MOTA
                    1743 CA
                                                    257 1.214 21.932 69.052 1.000 27.01
                                         SER
  ANISOU 1743 CA
                                          SER 257 2792
                                                                                 5165
                                                                                                     2304
                                                                                                                        109 -143 - 707
                                          SER 257 0.039 22.914 68.992 1.000 28.16
  MOTA
                    1744 CB
  ANISOU 1744 CB
                                       SER 257 2655 4473
                                                                                                     3572
                                                                                                                        -238 -90 -1071
  ATOM 1745 OG SER 257 0.491 24.251 69.074 1.000 51.32
ANISOU 1745 OG SER 257 8516 4131 6853 -616 -2734
                                                                                                     6853
                                                                                                                        -616 -2734 -807
                                         SER 257 2.259 22.389 68.034 1.000 26.19
                    1746 C
  MOTA
 ANISOU 1746 C SER 257 2537 5064 2350 -132 -413 -5
ATOM 1747 O SER 257 3.286 22.988 68.352 1.000 31.47
ANISOU 1747 O SER 257 2740 5886 3330 -435 -689 -6
                                                                                                                       -132 -413 -527
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1748 N ARG 258 2.022 22.123 66.763 1.000 26.04
1748 N ARG 258 3257 4477 2161 -238 -441 - 1
1749 CA ARG 258 2.982 22.541 65.747 1.000 25.81
1749 CA ARG 258 2.321 22.609 64.383 1.000 18.26
1750 C ARG 258 2.321 22.609 64.383 1.000 18.26
1750 C ARG 258 2.321 22.609 64.383 1.000 18.26
1751 O ARG 258 1.288 21.967 64.131 1.000 19.23
1751 O ARG 258 2600 2819 1888 -389 311 -4
1752 CB ARG 258 3403 5052 2861 695 -552 - 5
1753 CG ARG 258 4.246 20.784 64 384 1.000 32.664
                                                                                                                        -435 -689 -639
  ATOM
 ANISOU 1748 N
                                                                                                                        -238 -441 - 19
 ATOM
 ANISOU 1749 CA ARG
                                                                                                                        73 -338 -197.
 ATOM
 ANISOU 1750 C
 ATOM
 ANISOU 1751 O
                                                                                                                        -389 311 -420
 ATOM
 ANISOU 1752 CB ARG
                   1752 CB ARG 258 3403 5052 2861 695 -552 - 1753 CG ARG 258 4.246 20.784 64.384 1.000 32.64 1753 CG ARG 258 4358 4149 2006
                                                                                                                                     -552 - 57
 ATOM
 ANISOU 1753 CG ARG 258 4358
                                                                                  4148
                                                                                                     3896
                                                                                                                                      97 - 561
                                                                                                                        146
 ATOM 1754 CD ARG 258 5.325 19.746 64.499 1.000 30.38
ANISOU 1754 CD ARG 258 3812 4423 3309 -57 341 -
                                                                                                                                      341 - 16
                  1755 NE ARG 258 6.433 19.909 63.581 1.000 29.43
 ATOM
 ANISOU 1755 NE ARG 258 3990
                                                                                  4604
                                                                                                     2588
                                                                                                                        -22
                                                                                                                                       70 5 4 2
                  1756 CZ ARG
 ATOM
                                                     258 6.453 19.389 62.359 1.000 25.02
 ANISOU 1756 CZ ARG
                                                     258 2540
                                                                                 3893
                                                                                                    3074
                                                                                                                        304
                                                                                                                                      -243 1 0 4
 ATOM
                   1757 NH1 ARG
                                                     ANISOU 1757 NH1 ARG 258 2105 2607
                                                                                                   3982
                                                                                                                        359
ATOM 1758 NH2 ARG 258 7.523 19.593 61.617 1.000 22.03 ANISOU 1758 NH2 ARG 258 2477 2775 3120 -430 -287 -964 ATOM 1759 N THR 259 2.927 23.415 63.527 1.000 20.17 ANISOU 1759 N THR 259 2.010 3640 2013 -743 91 -1001 ATOM 1760 CA THR 259 2.485 23.505 62.138 1.000 18.33 ANISOU 1760 CA THR 259 1.821 24.821 61.713 1.000 23.23 ANISOU 1761 CB THR 259 1.821 24.821 61.713 1.000 23.23 ANISOU 1761 CB THR 259 2.839 25.830 61.681 1.000 34.27 ANISOU 1762 OG1 THR 259 2.839 25.830 61.681 1.000 34.27 ANISOU 1763 CG2 THR 259 2.181 2562 8277 -137 -996 -794 ATOM 1763 CG2 THR 259 4466 2233 2987 325 396 -948 ANISOU 1764 C THR 259 3.702 23.352 61.222 1.000 18.44 ANISOU 1765 O THR 259 3.702 23.352 61.222 1.000 18.44 ANISOU 1765 O THR 259 4.935 23.698 61.603 1.000 24.74 ANISOU 1766 N SER 260 3.420 ANISOU 1766 N SER 260 3.420 ANISOU 1766 N SER 260 1971 2352 1864 -224 2 -75 ATOM 1767 CA SER 260 1971 2352 1864 -224 2 -75 ATOM 1768 CB SER 260 1783 2961 1879 321 -95 -72 ATOM 1768 CB SER 260 1783 2961 1879 321 -95 -72 ATOM 1768 CB SER 260 5.224 21.514 58.956 1.000 20.17 ANISOU 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1768 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1769 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1769 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1769 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1769 CB SER 260 2306 3257 2100 762 -127 3 8 8 ATOM 1769 CB SER 260 2
                                                                                                                                       315 289
                   1758 NH2 ARG 258 7.523 19.593 61.617 1.000 22.03
 ATOM
                                                     260 5.224 21.514 58.956 1.000 20.17
260 2306 3257 2100 762 -127 3 8
260 4.416 20.392 58.698 1.000 27.09
 ANISOU 1768 CB SER
                                                                                                                        762 -127 3 8 8
 ATOM
                   1769 OG
                                        SER
 ANISOU 1769 OG SER 260 3651
                                                                                   2803
                                                                                                      3839 426
                                                                                                                                       217 554
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- 148 -
             1770 C
                          SER 260 3.832 23.062 57.614 1.000 14.52
 ATOM
                                                                                      -93 -1 2 5 7
                                                                                      -190 -120 - 500
                                                                                     -204 30 - 315
                                                                                     -42 -240 - 161
                                                                                     -68 -331 - 343
                                                                                     -399 -485 - 318
                                                                                     -719 -821 9 5 5
                                                                                     156 -103 1 7
ANISOU 1780 CB VAL 262 1262 1636 1614 9 -187 - 74
ATOM 1781 CG1 VAL 262 5.778 18.577 52.779 1.000 13.12
ANISOU 1781 CG1 VAL 262 1462 1527
ANISOU 1781 CG1 VAL 262 1462 1527 1997 -2 185 5 1
ATOM 1782 CG2 VAL 262 5.262 19.564 55.062 1.000 17.08
ANISOU 1782 CG2 VAL 262 3390 1494 1604 -374 -245 3
ATOM 1783 C VAL 262 5.096 21.149 51.543 1.000 11.18
ATOM 1784 O VAL 262 1026 1790 1431 1 -111 -13
ATOM 1784 O VAL 262 3.939 20.969 51.127 1.000 12.76
ANISOU 1784 O VAL 262 1064 2137 1648 -251 -84 -2
ATOM 1785 N PHE 263 6.090 21.438 50.714 1.000 9.50
ANISOU 1785 N PHE 263 995 1297 1316 -6 -210 -181
ATOM 1786 CA PHE 263 5.933 21.637 49.288 1.000 9.61
ANISOU 1786 CA PHE 263 1310 1017 1324 -6 -284 -4 2
ANISOU 1787 CB PHE 263 6.486 23.002 48.848 1.000 10.94
ANISOU 1787 CB PHE 263 6.486 23.002 48.848 1.000 10.94
ANISOU 1787 CB PHE 263 6.486 23.002 48.848 1.000 10.94
ANISOU 1787 CB PHE 263 6.56 150 23.399 47 418 1.000 10.35
                                                                        1997
                                                                                     -2 185 5 1
                                                                                     -374 -245 3 9
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263 6.150 23.399 47.418 1.000 10.35
ATOM
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                            PHE
ANISOU 1788 CG PHE
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            1789 CD1 PHE
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                                   ANISOU 1789 CD1 PHE
ATOM
            1790 CD2 PHE
ANISOU 1790 CD2 PHE
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            1791 CE1 PHE
ANISOU 1791 CE1 PHE
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263 4.769 24.601 45.836 1.000 13.12
                                                                                     31 - 370 136
            1792 CE2 PHE
ANISOU 1792 CE2 PHE
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                                                        1382
            1792 CE2 PRE 203 1431 1302 2131 43 -232 33.
1793 CZ PHE 263 5.491 24.112 44.762 1.000 12.42
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                                                                                    43 -292 353
ANISOU 1793 CZ PHE 263 1318
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                            PHE 263 6.636 20.505 48.530 1.000 8.91
ATOM
            1794 C
ANISOU 1794 C
                            PHE 263 1076
                           PHE 263 1076 1085 1223 -39 -1422
PHE 263 7.868 20.406 48.538 1.000 10.98
PHE 263 1098 1233 1842 -120 -224 -1
PHE 264 5.856 19.691 47.812 1.000 9.19
PHE 264 1089 1266 1136 -86 -105 -8
PHE 264 6.386 18.602 46.991 1.000 9.64
PHE 264 1009 1238 1417 -56 -60 -1
PHE 264 5.483 17.358 47.005 1.000 9.92
PHE 264 1209 1201 1359 -78 17 9
PHE 264 5.265 16.673 48.336 1.000 11.22
PHE 264 1241 1647 1374 -121 38 7 7
PHE 264 6.292 16.236 49.139 1.000 15.38
                                                        1085
                                                                       1223
                                                                                     -39 -142 2 4
            1795 0
MOTA
ANISOU 1795 O
                                                                                     -120 -224 -145
            1796 N
MOTA
ANISOU 1796 N
                                                                                     -86 -105 - 82
            1797 CA
ATOM
ANISOU 1797 CA
                                                                                     -56 -60 -126
            1798 CB
ANISOU 1798 CB
            1799 CG
ANISOU 1799 CG
MOTA
            1800 CD1 PHE
                                                       16.236 49.139 1.000 15.38
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- 149 -ANISOU 1800 CD1 PHE 264 1467 2641 1734 -225 -8 8 7 3 1801 CD2 PHE ATOM 264 3.988 16.433 48.808 1.000 16.96 ANISOU 1801 CD2 PHE 264 1425 3252 1769 -610 -79 958 1802 CE1 PHE ATOM 264 6.090 15.596 50.336 1.000 14.52 ANISOU 1802 CE1 PHE 264 1745 1354 2417 162 334 452 1803 CE2 PHE 264 3.755 15.796 50.019 1.000 18.04 ANISOU 1803 CE2 PHE 264 1747 3405 1704 -590 -109 1008 MOTA 1804 CZ PHE 264 4.817 15.354 50.779 1.000 12.52 ANISOU 1804 CZ PHE 264 1772 1536 1449 -57 227 3 19.038 45.533 1.000 8.98 227 334 1805 C ATOM PHE 264 6.535 ANISOU 1805 C PHE 264 1103 919 1392 143 81 - 92 1806 O PHE 19.368 44.930 1.000 9.79 264 5.497 ANISOU 1806 O PHE 264 991 1190 1540 28 105 1 0 3 1807 N LEU 265 7.758 19.031 44.999 1.000 8.43 ANISOU 1807 N LEU 265 992 884 1325 1808 CA LEU 265 7.984 MOTA ANISOU 1808 CA LEU 265 883 1066 1339 63 -33 1809 CB LEU 265 9.309 19.964 43.328 1.000 10.10 ATOM ANISOU 1809 CB LEU 265 1179 1188 1469 -225 -220 2 4 8 1810 CG ATOM LEU 265 9.570 20.351 41.871 1.000 9.37 ANISOU 1810 CG LEU 265 1072 1009 1478 242 1811 CD1 LEU 265 8.725 21.522 41.408 1.000 10.80 ANISOU 1811 CD1 LEU 265 1291 1.004 1811 181 -114 2 9 6 1812 CD2 LEU 265 11.048 20.684 41.678 1.000 10.87 ANISOU 1812 CD2 LEU 265 1129 1483 1519 134 43 14 (ATOM 1813 C LEU 265 7.933 17.849 42.875 1.000 10.21 134 43 1 4 6 ANISOU 1813 C LEU 265 932 1188 1760 -6 -38 -302 LEU 265 8.858 17.043 43.042 1.000 10.45 LEU 265 1388 969 1612 84 -217 107 ATOM 1814 0 ANISOU 1814 O 969 1612 84 -217 107 266 6.853 17.530 42.135 1.000 10.00 1815 N ATOM ARG ANISOU 1815 N ARG 1816 CA ATOM ARG ANISOU 1816 CA ARG 1817 CB ARG ARG 266 978 1460 1574 -168 -103 -105 ARG 266 4.965 15.894 43.609 1.000 11.24 ANISOU 1817 CB 1818 CG ANISOU 1818 CG 266 1337 ARG MOTA 1819 CD ARG 266 3.668 ANISOU 1819 CD ARG 266 1113 ARG 266 1113 1567 1564 -17 -49 -ARG 266 2.508 15.879 43.447 1.000 9.43 -17 -49 -11MOTA 1820 NE 1821 CZ ARG 266 1.236 15.509 43.657 1.000 9 . 4 3 1821 CZ ARG 266 1.245 15.509 43.657 1.000 9 . 8 3 1822 NH1 ARG 266 0.961 14.567 44.572 1.000 11.20 1822 NH1 ARG 266 1208 1240 1806 -144 -454 2 7 3 1823 NH2 ARG 266 0 225 16 000 ANISOU 1820 NE ATOM ANISOU 1821 CZ ARG 266 1245 MOTA ANISOU 1822 NH1 ARG 266 1208 -144 -454 2 7 2 1823 NH2 ARG 266 0.225 16.048 42.975 1.000 11.08 ANISOU 1823 NH2 ARG 266 1460 1265 1484 191 -283 7 ATOM 1824 C ARG 266 6.601 16.190 40.099 1.000 10.28 ANISOU 1824 C ARG 266 1273 1089 1545 -200 -5 -16 191 -283 7 3 -200 -5 -167 ATOM 1825 O ARG 266 6.027 17.109 39.519 1.000 11.05 ANISOU 1825 O ARG 266 1254 1153 1793 -132 47 - 64 PRO 267 7.215 15.162 39.496 1.000 10.27 ATOM 1826 N ANISOU 1826 N PRO 267 1194 1239 1468 -33 130 3 2 MOTA PRO 267 7.828 1827 CD 13.963 40.109 1.000 12.36 ANISOU 1827 CD PRO 267.1865 1132 1697 -26 -529 - 192 ATOM 1828 CA PRO 267 7.304 15.157 38.036 1.000 10.12 ANISOU 1828 CA PRO 267 1278 1095 1472 -129 38 - 185 ATOM 1829 CB PRO 267 8.250 13.986 37.767 1.000 11.83 ANISOU 1829 CB PRO 267 1489 1088 1919 -72 90 - 322 MOTA 1830 CG PRO 267 8.017 13.053 38.913 1.000 10.72 ANISOU 1830 CG PRO 267 960 1356 1755 95 - 257 - 187

						- 150 -		
ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU	11111111111111111111111111111111111111	COONNAABBGGDDDCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	NNNNNAAAAALAAAASSSSSSSSSSSSSSSSSSSSSSSS	22222222222222222222222222222222222222	1216 4.810 1285 4.954 2160 4.999 1811 4.999 18.046 1910 6.037 25.715 15.34 14.129 15.715 14.32 17.432 17.432 17.432 17.432 17.432 17.432 17.433 14.453 15.443 17.443	-150- 14.26 14.26 14.26 14.26 14.17 15.26 114.99 15.16 14.99 15.17 17.39 174.81 177.31 174.81 177.31 174.81 177.31 174.81 177.31 174.81 177.31 174.81 177.31 174.81 177.31 174.81 177.31 174.81 177.31 174.81	1570 37.934 2080 36.065 1670 38.198 1622 1756 31.4756 31.5985 31.	-258 17 7 7 1.000 10.61 -70
ATOM ANISOU ATOM ANISOU ATOM ANISOU ANISOU	1857 1857 1858 1858 1859 1859	CG CD1 CD1 CD2 CD2	PHE PHE PHE PHE PHE	271271271271271	10.385 1411 11.475	11.992 1640 12.488	34.597 1800 33.904	1.000 12.77 42 31 5 6 1.000 13.22 168 220 4 9 1.000 13.55
ATOM ANISOU ATOM	1860	CE1	PHE PHE	271 271	12.779 1432 11.925	12.178 1760 10.806	34.249 2225 36.019	139 84 2 5 5 1.000 14.26 -39 46 - 4 1 6 1.000 15.88

								16176070703000
						- 151 -		
ANISOU	1861	CE2			1537	1818	2679	-263 -675 2 6 0
ATOM	1862		PHE		13.006	11.288	35.304	1.000 14.15
ANISOU			PHE		1166	1736	2475	7 -531 -467
MOTA	1863		PHE		9.259	10.550	32.410	1.000 11.27
ANISOU			PHE		1359	1338	1585	75 271 3 4 8
ATOM	1864		PHE		8.785	9.531	32.920	1.000 12.97
ANISOU			PHE	271	2011	1320	1596	-85 473 279
ATOM	1865	N	THR	272	10.261	10.498	31.541	1.000 11.95
ANISOU			THR	272	1018	1503	2020	-214 300 -115
ATOM	1866		THR		10.823	9.254	30.992	1.000 12.70
ANISOU			THR		1615	1557	1652	132 341 146
ATOM	1867		THR		10.679	9.281	29.450	1.000 16.79
ANISOU			THR	272	1814	2829	1737	-595 157 -406
ATOM	1868				9.301	9.471	29.090	1.000 18.02
ANISOU		OG1			1912	2921	2013	-497 -73 9 1
ATOM ANISOU	1869	CG2	THR	272	11.200	7.976	28.856	1.000 17.02
					2144	2857	1467	-475 538 -194
ATOM ANISOU	1870		THR		12.272	9.057	31.423	1.000 12.02
ATOM	1871		THR		1436	1573	1559	92 603 1 3 7
ANISOU		0	THR		13.055	10.031	31.437	1.000 14.17
ATOM	1872	N	THR PHE	272	1451	1583	2351	125 602 412
ANISOU		N	PHE	273 273	12.625	7.837	31.828	1.000 12.34
ATOM	1873		PHE	273	1402 13.953	1585	1703	17 378 1 5 8
ANISOU			PHE		1362	7.492	32.312	1.000 12.20
ATOM	1874		PHE	273		1364 7.514	1909	-126 336 147
ANISOU			PHE	273	1362	1447	33.861 1890	1.000 12.37 -102 211 - 8
ATOM	1875		PHE		12.988	6.528	34.491	
ANISOU	1875	ĊĠ	PHE		1398	1631	1396	1.000 11.65 -367 42 - 215
ATOM	1876		PHE	273	11.684	6.889		1.000 14.11
ANISOU	1876	CD1	PHE	273	1531	2214	1614	-336 293 - 62
ATOM	1877	CD2	PHE		13.409	5.245	34.803	1.000 13.20
	1877	CD2	PHE	273		1639	1352	-358 339 - 9
ATOM	1878	CE1	PHE	273	10.793	5.993	35.323	1.000 13.25
ANISOU	1878	CE1	PHE	273	1536	2081	1418	-98 447 4 2
ATOM	1879	CE2	PHE	273	12.530	4.329	35.327	1.000 13.39
		CE2		273	1529	1905	1654	-224 140 283
ATOM		CZ	PHE	273	11.227	4.706		1.000 14.75
ANISOU			PHE	273	1444	2260	1902	-90 -186 2 7 5
ATOM	1881		PHE		14.423	6.135		1.000 12.45
ANISOU			PHE	273	1278	1526	1927	-120 317 - 31
ATOM			PHE		13.645	5.311	31.291	1.000 11.95
ANISOU ATOM			PHE		1590	1580	1370	-137 226 - 13
ANISOU	1883	IV N	SER		15.717	5.854	31.952	1.000 12.07
ATOM	1884		SER		1270	1640	1677	-29 558 353
ANISOU			SER		16.335	4.586	31.604	1.000 14.39
ATOM	1885	CB	SER SER		1583	1534	2349	43 707 3 8 4
ANISOU		CB	SER	274	17.845 1578	4.771		1.000 14.49
ATOM	1886		SER	274	18.564	1727	2202	213 695 3 2 9
ANISOU	1886	06	SER		1763	3.558	31.424	1.000 14.97
ATOM	1887	C	SER		16.100	1848	2078	349 348 - 1 3
ANISOU		C	SER		1670	3.505 1481		1.000 13.12
ATOM	1888	0	SER	274	16.438	3.700	1833	8 461 137
ANISOU		Ö	SER	274	1493	1518	33.834 2116	1.000 13.50
ATOM	1889	N	VAL		15.533	2.359		-65 119 1 5 1.000 11.90
ANISOU			VAL	275	1476	1618	1427	
ATOM	1890		VAL		15.283	1.254	33.180	-110 490 195 1.00011.41
ANISOU	1890		VAL	275	1708	1424	1204	-8 286 7 6
ATOM	1891	CB	VAL	275	14.346	0.198		1.000 12.74
ANISOU			VAL	275	1732	1300	1809	62 164 - 1 6
				5	_ ,	1300	1003	07 TO4 - T D

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- 152 -
             1892 CG1 VAL 275 14.157 -1.020 33.437 1.000 16.10
 MOTA
             1892 CG1 VAL 275 2352 1803 1962
1893 CG2 VAL 275 12.961 0.763 32.261
275 1535 1786 1924
 ANISOU 1892 CG1 VAL 275 2352
                                                                                     -614 -663 3 7 0
                                                                       32.261 1.000 13.81
 ANISOU 1893 CG2 VAL 275 1535
                                                                                     16 363 126
                                     275 16.577 0.622 33.692 1.000 12.62
             1894 C
 MOTA
                            VAL
 ANISOU 1894 C
                                     275 1574
                             VAL
                                                                      1594
                                                          1628
                                                                                     14 375 1 3 6
                                     275 16.729 0.405 34.926 1.000 13.01
 MOTA
             1895 0
                            VAL
 ANISOU 1895 O
                            VAL
                                     275 1667 1643
                                                                      1634
                                                                                    9 113 180
             1896 N
 ATOM
                            PRO
                                     276 17.569 0.286 32.889 1.000 14.64
 ANISOU 1896 N
                            PRO
                                    276 1583 2066
                                                                      1914
                                                                                    2 454 - 42
 ATOM 1897 CD PRO
ANISOU 1897 CD PRO
                                    276 17.583 0.285 31.415 1.000 15.84
                                    276 1565 2536 1916 89 755 3 5
276 18.827 -0.250 33.453 1.000 16.76
276 1667 2403 2296 261 393 -
             1898 CA
 ATOM
                           PRO
ANISOU 1898 CA PRO 276 1667 2403 2296 261 393 -1 ATOM 1899 CB PRO 276 19.732 -0.503 32.236 1.000 18.27 ANISOU 1899 CB PRO 276 1804 2568 2571 411 574 -1 ATOM 1900 CG PRO 276 18.868 -0.385 31.029 1.000 18.96 AIISOU 1900 CG PRO 276 19.500 0.710 34.420 1.000 16.32 ANISOU 1901 C PRO 276 1521 2342 2336 11.5 237 6 7 ANISOU 1902 O PRO 276 20.035 0.277 35.456 1.000 16.78 ANISOU 1902 O PRO 276 1411 2689 2275 93 376 253 ATOM 1903 N LEU 277 19.475 2.019 34.155 1.000 16.58 ANISOU 1903 N LEU 277 1835 2412 2052 -15 483 14 ANISOU 1904 CA LEU 277 1990 2226 2511 -21 362 11 ATOM 1905 CB LEU 277 20.142 2.919 35.099 1.000 17.70 ANISOU 1904 CA LEU 277 20.142 2.919 35.099 1.000 17.70 ANISOU 1905 CB LEU 277 20.298 4.277 34.425 1.000 20.20 ANISOU 1905 CB LEU 277 2952 2292 2432 -1 -14 271 ATOM 1906 CG LEU 277 21.048 5.359 35.186 1.000 20.86 ANISOU 1907 CD1 LEU 277 22.446 4.888 35.531 1.000 34.24 ANISOU 1907 CD1 LEU 277 21.062 6.620 34.334 1.000 31.91
 ANISOU 1898 CA
                            PRO
                                                                                    261 393 -163
                                                                                            574 - 142
                                                                                            694 - 37
                                                                                              237 6 7
                                                                                             483 148
                                                                                    -21 362 118
                                                                                    -32 -355 4 8 2
ATOM 1908 CD2 LEU 277 21.062 6.620 34.334 1.000 31.91
ANISOU 1908 CD2 LEU 277 4745 2460 4918 -474 -572 1
                                                                                    -474 -572 1150
            1909 C LEU 277 19.411 2.989 36.430 1.000 16.55
1909 C LEU 277 1975 1885 2430 -218 211 -243
ANISOU 1909 C
 ANISOU 1918 CB
                           ARG
                                     279 1889 1897 2609 84 544 2 5 0
279 16.790 -2.323 37.291 1.000 19.63
                                     279 1889
             1919 CG
 ATOM
                            ARG
 ANISOU 1919 CG
                                    279 2123 2196 3139 -63 233 9
279 16.656 -3.288 36.131 1.000 27.03
                           ARG
                                                                                    -63 233 9 1
 ATOM
             1920 CD
                           ARG
 ANISOU 1920 CD
                                    279 3924 3198 3150 -603 -275 - 279 17.236 -4.578 36.364 1.000 27.45
                           ARG
                                                                                    -603 -275 -198
 ATOM
             1921 NE
                           ARG
 ANISOU 1921 NE ARG 279 4659
                                    279 4659 2854 2915 -359 751 -789
279 16.714 -5.717 36.779 1.000 32.85
 ATOM
             1922 CZ
                           ARG
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ANISOU 1922 CZ ARG
                    279 4486
                                3045
                                        4948
                                               -475 448 -222
       1923 NH1 ARG
                    279 15.424
                                -5.874 37.089 1.000 29.96
ANISOU 1923 NH1 ARG
                    279 4653
                                2168
                                       4562
                                               -103 967 -678
       1924 NH2 ARG
                    279 17.551
                                -6.750 36.890 1.000 37.87
ANISOU 1924 NH2 ARG
                    279 4879
                                2436
                                       7074
                                               -276 3273 - 824
MOTA
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               ARG
                    279 19.628
                                -0.519 39.150 1.000 17.48
                    279 2118
ANISOU 1925 C
               ARG
                                1653
                                       2871
                                               75 -8 705
ATOM
       1926 0
                    279 19.916
               ARG
                                -1.064 40.212 1.000 26.82
ANISOU 1926 O
                    279 3764
               ARG
                                3102
                                        3325
                                               -1987 -1467 1383
MOTA
       1927 N
               GLU
                    280 20.538
                                0.189
                                       38.505 1.000 17.73
ANISOU 1927 N
               GLU
                    280 1983
                                2293
                                       2459
                                               109
                                                     609 3 7
MOTA
       1928 CA
               GLÜ
                    280 21.899
                                0.317
                                       39.026 1.000 19.66
ANISOU 1928 CA
               GLU
                    280 2049
                                2023
                                               125
                                        3396
                                                     215 737
MOTA
       1929 CB
               GLU
                    280 22.836
                                0.886
                                        37.936 1.000 20.17
ANISOU 1929 CB
               GLU
                    280 1648
                                2457
                                        3560
                                               464
                                                     138 1099
ATOM
       1930 CG
                    280 22.964
                               -0.149 36.818 1.000 31.79
               GLU
                    280 3477 4175
ANISOU 1930 CG
               GLU
                                       4427
                                               801
                                                     1187 - 4
ATOM
       1931 CD
                    280 23.698
               \operatorname{\mathsf{GLU}}
                                0.341
                                       35.590 1.000 39.66
ANISOU 1931 CD
               GLU
                    280 5144
                                5703
                                       4221
                                               -64
                                                     1339 - 6
       1932 OE1 GLU
MOTA
                    280 24.466
                               1.327
                                       35.685 1.000 39.65
ANISOU 1932 OE1 GLU
                   280 3464
                                5891
                                       5710
                                               334
                                                     574 1639
MOTA
       1933 OE2 GLU
                               -0.294 34.519 1.000 41.55
                   280 23.489
ANISOU 1933 OE2 GLU
                   280 5257
                                6747
                                       3781
                                               2245 -184 1 0 2
ATOM
       1934 C
               GLU
                    280 21.984
                                1.188
                                       40.266 1.000 19.68
ANISOU 1934 C
               GLU
                    280 1488
                                2350
                                       3640
                                               -566 162 490
       1935 O
MOTA
                    280 23.031 1.142
               GLU
                                       40.958 1.000 25.69
ANISOU 1935 O
               GLU
                    280 1871
                                3766
                                       4123
                                               231
                                                     -245 1 8 0
ATOM
      1936 N
               CYS
                    281 20.943 1.980
                                       40.565 1.000 18.57
ANISOU 1936 N
               CYS
                    281 1560
                                2609
                                               -406 -211 1 7 6
                                       2887
MOTA
      1937 CA
               CYS
                    281 21.098 2.762
                                       41.806 1.000 23.83
ANISOU 1937 CA
               CYS
                    281 3222
                                2647
                                       3184
                                               -1189 176 -122
      1938 CB
ATOM
               CYS
                    281 21.079
                               4.264
                                       41.523 1.000 25.40
ANISOU 1938 CB
               CYS
                    281 3278
                                2655
                                       3718
                                               -426 368 - 46
      1939 SG
ATOM
               CYS
                    281 19.587
                               4.904
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ANISOU 1939 SG
               CYS
                    281 3069
                                2914
                                       4295
                                               -522 -37 -794
      1940 C
ATOM
               CYS
                    281 20.098
                                2.406
                                       42.907 1.000 16.99
ANISOU 1940 C
               CYS
                    281 1377
                                1604
                                       3475
                                               109 -6 -546
ATOM
      1941 0
               CYS
                    281 19:971
                                3.173
                                       43.889 1.000 17.04
ANISOU 1941 O
               CYS
                    281 2294
                                1277
                                       2902
                                               -204 -484 -129
ATOM
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               GLY
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                                1.245
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ANISOU 1942 N
               GLY
                    282 1617
                                1597
                                       2572
                                               3 -58 -436
ATOM
      1943 CA
               GLY
                    282 18.731
                                0.674
                                       43.914 1.000 15.61
ANISOU 1943 CA
                    282 1565
               GLY
                                1973
                                       2394
                                               6 -331 -266
      1944 C
ATOM
                    282 17.246
               GLY
                                0.519
                                        43.727 1.000 13.75
ANISOU 1944 C
               GLY
                    282 1635
                                1562
                                       2029
                                               -270
                                                    -446 - 78
      1945 0
ATOM
               GLY
                    282 16.585
                                0.012
                                       44.639 1.000 14.99
ANISCU 1945 O
               GLY
                    282 1751
                                1630
                                       2313
                                               207
                                                     -242 4 5 5
      1946 N
               PHE
                    283 16.744
                                       42.582 1.000 12.65
                                1.009
ANISOU 1946 N
               PHE
                    283 1434
                                1803
                                       1570
                                               -200 18 - 252
      1947 CA
ATOM
               PHE
                   283 15.292
                                0.886
                                       42.374 1.000 11.80
ANISOU 1947 CA
               PHE 283 1477
                                1032
                                       1974
                                               -15
                                                   -264 4 6
ATOM
      1948 CB
               PHE
                   283 14.839
                                       41.295 1.000 14.13
                                1.890
ANISOU 1948 CB
               PHE 283 2262
                                972 2136 109
                                                -187 159
ATOM
               PHE
      1949 CG
                   283 14.906
                                3.351
                                      41.757 1.000 12.63
ANISOU 1949 CG
               PHE 283 1711
                                1033
                                       2055
                                               47 -86 9
ATOM
      1950 CD1 PHE
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ANISOU 1950 CD1 PHE
                    283 1697
                                1399
                                       2013
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MOTA
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ANISOU 1951 CD2 PHE
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ATOM
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                    283 13.903
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ANISOU 1952 CE1 PHE
                    283 2111
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                                        2171
                                               -202 484 -617
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- 154 -
           1953 CE2 PHE 283 16.112 5.432 41.963 1.000 12.60
 ANISOU 1953 CE2 PHE
                               283 1783
                                               937 2068 32 -18
          1954 CZ PHE
                               283 15.040 5.993 42.641 1.000 13.37
 ANISOU 1954 CZ PHE
                               283 1863
                                               865 2352 187 -149 1 3
           1955 C PHE
                               283 14.915
                                               -0.534 41.972 1.000 11.23
 ANISOU 1955 C
                       PHE
                               283 1527
                                               974 1765 63 -172 6 5
          1956 0
 ATOM
                       PHE
                               283 15.471
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 ANISOU 1956 O
                               283 1249
                       PHE
                                               1428 2355 175 -120 - :
-1.130 42.712 1.000 12.31
                                                                    175 -120 - 361
         1957 N
 ATOM
                       ASP
                               284 13.998
 ANISOU 1957 N
                       ASP 284 1607
                                               1333
                                                          1736
                                                                    -268 -312 8 7
        1958 CA ASP 284 13.589 -2.528 42.527 1.000 12.48
 ATOM
 ANISOU 1958 CA ASP 284 1725
                                               1202
                                                          1814
                                                                    -148 -543 3 5 0
          1959 CB ASP
 ATOM
                              284 13.159 -3.156 43.876 1.000 12.67
 ANISOU 1959 CB ASP
                               284 2014
                                               1145
                                                          1656
                                                                     -50 -406 1 3 5
 ATOM 1960 CG ASP 284 13.261 -4.667 43.909 1.000 13.40 ANISOU 1960 CG ASP 284 2077 1171 1843 110 -419 3
                                                                     110 -419 3 6 3
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 ATOM
ANISOU 1962 OD2 ASP
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ANISOU 1963 C
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MOTA
          1964 0
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ANISOU 1964 O
                       ASP
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          1965 N
ATOM
                              285 12.751 -2.154 40.308 1.000 11.32
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ANISOU 1965 N VAL 285 1204 1671 1426 -93 -48 6 1
ATOM 1966 CA VAL 285 11.748 -2.062 39.260 1.000 11.45
ANISOU 1966 CA VAL 285 1468 1384 1500 39 -219 - 15
ANISOU 1967 CB VAL 285 12.153 -1.072 38.157 1.000 11.58
ANISOU 1967 CB VAL 285 1412 1523 1465 -388 -428 - 8
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ANISOU 1968 CG1 VAL 285 2209 1458 2040 -264 -442 - 32
ATOM 1969 CG2 VAL 285 13.467 -1.482 37.495 1.000 15.70
ANISOU 1969 CG2 VAL 285 1909 1443 2615 -159 309 4 4 7
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ANISOU 1971 O VAL 285 12267 -4.301 38.520 1.000 12.13
ANISOU 1971 O VAL 285 1214 1192 2202 -28 300 162
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ANISOU 1973 CA SER 286 9.558 -4.622 37.510 1.000 11.32
ANISOU 1973 CA SER 286 9.558 -4.622 37.510 1.000 11.32
ANISOU 1973 CA SER 286 1104 1479 1718 -41 -274 2 5 2
ANISOU 1965 N
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ANISOU 1973 CA SER 286 1104 1479 1718 -41 -274 2 9 1700 1974 CB SER 286 8.483 -5.292 38.344 1.000 9.88 ANISOU 1974 CB SER 286 1328 1141 1285 72 -207 7 0 ANISOU 1975 OG SER 286 7.570 -4.361 38.905 1.000 11.34 ATOM 1976 C SER 286 9.019 -4.106 36.175 1.000 10.34 ANISOU 1976 C SER 286 9.019 -4.106 36.175 28 -87 2 4 5
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ANISOU 1976 C
ATOM 1977 O
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SER 286 7.829 -4.112 35.869 1.000 12.62
ANISOU 1977 O
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ANISOU 1978 N
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                       LEU
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ANISOU 1979 CA
                      LEU
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                                                          1605
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ANISOU 1980 CB
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                                                          1597
                                                                     -373 - 95 2 7
          1981 CG
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ANISOU 1981 CG LEU
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                                                                    -407 -51 -170
          1982 CD1 LEU
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ANISOU 1982 CD1 LEU
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ATOM
          1983 CD2 LEU
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- 155 -

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                                                                                                                                                                   THR 291 1863 1604 1421 47 305 2 1 9
THR 291 10.625 2.024 29.270 1.000 16.13
THR 291 2344 1983 1804 -303 750 -431
        ANISOU 2012 C
        ATOM
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       ANISOU 2013 O
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 292
 1362
 1257
 1779
 -213
 153
 3

 292
 9.718
 2.954
 32.439
 1.000
 12.62
 -213 153 3 7 MOTA 2016 CB ALA292 1768 1245 1784 100 357 4 292 9.385 5.255 31.614 1.000 10.32 ANISOU 2016 CB ALAMOTA 2017 C ALAANISOU 2017 C ALA 292 9.385 5.255 31.614 1.000 10.32 ANISOU 2018 O ALA 292 10.266 6.134 31.701 1.000 10.97 ANISOU 2018 O ALA 292 1389 1138 1641 -146 279 10 ATOM 2019 N THR 293 8.091 5.445 31.882 1.000 12.32 ANISOU 2019 N THR 293 1486 1547 1647 -314 563 -2 ATOM 2020 CA THR 293 7.626 6.715 32.421 1.000 12.28 ANISOU 2020 CA THR 293 1717 1460 1489 -168 337 -2 ATOM 2021 CB THR 293 6.352 7.215 31.733 1.000 13.27 ANISOU 2021 CB THR 293 2128 1182 1730 -258 -159 -2 ATOM 2022 OG1 THR 293 5.317 6.237 31.011 1.000 13.27 -146 279 104 -314 563 - 284 -168 337 -200 -258 -159 - 284 -252 -56 -405 THR 293 7.363 6.635 33.937 1.000 10.58 THR 293 1439 1050 1533 12 447 9 ATOM 2024 C THR 293 7.363 6.635 33.937 1.000 10.58 ANISOU 2024 C THR 293 1439 1050 1533 12 447 9 ATOM 2025 O THR 293 1049 1102 1758 -56 93 118 ATOM 2026 N PHE 294 7.243 7.810 34.569 1.000 10.29 ANISOU 2026 N PHE 294 1794 1093 1494 -307 306 -66 ATOM 2027 CA PHE 294 6.806 7.939 35.950 1.000 10.41 ATOM 2027 CA PHE 294 1432 1061 1463 -174 125 -162 ATOM 2028 CB PHE 294 1432 1061 1463 -174 125 -162 ATOM 2028 CB PHE 294 1930 1030 1694 -164 292 -64 ATOM 2029 CG PHE 294 1880 1136 1837 -103 178 -427 ANISOU 2029 CG PHE 294 1880 1136 1837 -103 178 -427 ANISOU 2030 CD1 PHE 294 1880 1136 1837 -103 178 -427 ATOM 2030 CD1 PHE 294 1976 1893 1727 -539 161 -132 ATOM 2031 CD2 PHE 294 4.989 10.068 38.056 1.000 16.59 ANISOU 2031 CD2 PHE 294 4.989 10.068 38.056 1.000 16.59 ANISOU 2032 CE1 PHE 294 2180 1923 2199 348 386 -492 ATOM 2032 CE1 PHE 294 1598 2028 1830 -505 280 -118 ATOM 2033 CE2 PHE 294 1598 2028 1830 -505 280 -118 ATOM 2033 CE2 PHE 294 2214 2062 2087 692 144 -602 ATOM 2034 CZ PHE 294 2214 2062 2087 692 144 -602 ATOM 2035 C PHE 294 2214 2062 2087 692 144 -602 ATOM 2035 C PHE 294 2484 7.195 36.172 1.000 10.67 ANISOU 2035 C PHE 294 2484 7.195 36.172 1.000 10.67 ATOM 2036 O PHE 294 1401 1200 1536 -155 78 13 7 ANISOU 2035 C PHE 294 4.884 7.195 36.172 1.000 10.67 ATOM 2037 N GLN 295 1399 1187 1450 -18 88 -24 ATOM 2037 N GLN 295 1399 1187 1450 -18 88 -24 ATOM 2038 CA GLN 295 3.217 6.6612 35.393 1.000 11.31 ATOM 2024 C ANISOU 2024 C -18 88 - 24 ATOM 2038 CA GLN 295 1433 1205 1660 -96 120 -3 295 2.284 7.053 34.254 1.000 11.66 295 1425 1053 1953 -25 63 -14 ANISOU 2038 CA GLN-96 120 -321 MOTA 2039 CB GLNANISOU 2039 CB GLNATOM 2040 CG GLN 295 1425 1053 1953 -25 63-14
ATOM 2040 CG GLN 295 0.951 6.360 34.200 1.000 11.05
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ATOM 2041 CD GLN 295 0.052 6.843 33.087 1.000 11.35
ANISOU 2041 CD GLN 295 1592 1326 1395 173 57 - 13
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ANISOU 2042 OE1 GLN 295 2306 1589 1825 - 110 7 3 7 9
ATOM 2043 NE2 GLN 295 -1.053 6.153 32.914 1.000 13.90
ANISOU 2043 NE2 GLN 295 1511 1757 2015 156 -282 2 (
ATOM 2044 C GLN 295 3.412 5.107 35.389 1.000 10.12 -25 63 - 141 -93 -118 1 8 173 57 - 1 3 182,5 - 110 7 3 7 9 156 -282 2 0 8

								1 6 17 6 27 6, 62 60 6
						- 157 -		
ANISOU 2			GLN		1154	1203	1486	21 160 - 191
	2045		GLN		2.827	4.309	36.128	1.000 11.32
ANISOU 2			GLN		1264	1542	1686	-107 41 137
	2046		ASP		4.267	4.558	34.538	1.000 9 . 3 5
ANISOU 2			ASP		1076	1056	1422	-118 -75 -275
	2047		ASP		4.655	3.172	34.416	1.000 9 . 9 1
ANISOU 2			ASP		1241	1139	1387	56 60 - 243
		CB	ASP		5.699	2.852	33.347	1.000 10.26
ANISOU 2			ASP		1315	1156	1429	113 132 - 36
	2049		ASP		5.343	2.981	31.885	1.000 11.42
ANISOU 2	2050		ASP	296	1357	1578	1405	358 121 - 199
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	2053		ASP		4.852	1.551	36.197	1.000 11.40
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ATOM 2	2054	N	TRP		6.004	3.484	36.441	1.000 10.88
ANISOU 2			TPP		1752	1144	1238	-161 11 5 5
	2055		TRP	297		3.104	37.685	1.000 11.26
ANISOU 2			TRP		1768	1215	1294	-217 -57 4 5
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ANISOU 2			TRP		1387	1417	1112	-87 213 120
ATOM 2 ANISOU 2	2057		TRP		8.621	3.651	39.172	1.000 10.98
	2057		TRP		1456	1394	1324	164 -29 -43
ANISOU 2	2058	CD2	TRP		9.082 1255	4.534 1729	40.202 1761	1.000 12.49
ATOM 2	2059	CE2	TRP	297		3.755	41.201	75 -298 -197 1.000 16.08
ANISOU 2	2059	CE2	TRP		1860	2049	2202	-294 -977 4 9
ATOM 2	2060	CE3	TRP		9.040	5.910	40.379	1.000 17.41
ANISOU 2					2778	1740	2096	-388 -916 - 234
ATOM 2	2061	CD1	TRP	297	8.969	2.400	39.589	1.000 13.58
ANISOU 2	2061	CD1	TRP		1617	1518	2025	0 -664 114
ATOM 2	2062	NEl	TRP	297	9.614	2.444	40.808	1.000 16.12
ANISOU 2				297		1909	2051	-22 -873 2 2 0
ANISOU 2	2063	CZZ	TKP	29/	10.243	4.320	42.341	1.000 19.85
ATOM 2	2064	CZZ	455 175		2756 9.586	2383 6.466	2404	-951 -1337 267
ANISOU 2	2064	CZ3	ጥጽኮ		4215	2030	41.515 2645	1.000 23.40 -1001 -1757 - 77
	2065				10.181	5.670	42.486	1.000 21.51
ANISOU 2	2065	CH2	TRP		3178	2457	2537	-910 -1473 - 51
ATOM 2	2066	С	TRP		5.700	3.138	38.882	1.000 10.39
ANISOU 2			TRP		1172		1329	-280 -237 3 9 1
	2067		TRP		5.574	2.159	39.639	1.000 13.52
ANISOU 2			TRP		1748	1830	1557	32 -91 7 0 3
	2068		ILE		5.033	4.272	39.079	1.000 12.08
ANISOU 2			ILE		1400	1710	1480	-49 83 4 5 1
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	2070		ILE ILE		1301	2484	1317	-199 -158 - 3 3
	2070		ILE		4.370 1877	5.988	.40.689	1.000 16.97
	2071		ILF		3.538	2908 6.423	1661 41.876	-1000 214 -630 1.000 22.01
ANISOU 2	2071	CG2	ILE		3980	3121	1263	-233 546 -339
ATOM 2	2072	CG1	ILE		5.847	6.253	41.037	1.000 27.10
ANISOU 2	2072	CG1	ILE	298	2588	5151	2557	-2140 -708 9 7
ATOM 2	2073	CD1	ILE	298	6.365	5.522	42.266	1.000 43.13
ANISOU 2				298	5185	8299	2904	-3717 -3055 7 0 8
	2074		ILE		2.772	4.116	40.131	1.000 10.94
ANISOU 2	20/4	C	ILE	298	1350	1652	1156	-165 -79 9 6

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- 158 -
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                   ILE 298 2.137
                                      3.844
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ANISCU 2075 O
ATOM 2076 N
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ATOM
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ANISOU 2083 O
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                  ASN
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ATOM
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ATOM 2087 CG
ANISOU 2087 CG
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ATOM
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                  TYR
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ANISOU 2093 CA
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        2094 CB
ATOM
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ATOM
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ATOM
       2105 CA VAL
                        303 2.309 8.430 45.820 1.000 11.88
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- 159 -ANISOU 2105 CA VAL 303 1434 1609 1471 -368 -197 2 2 3 2106 CB VAL 303 2.755 6.967 45.736 1.000 14.57 ANISOU 2106 CB VAL 303 1395 1682 -217 -918 3 1 2 2459 2107 CG1 VAL 303 3.131 6.462 47.132 1.000 17.33 ANISOU 2107 CG1 VAL 303 2644 1608 2331 -48 -1114 6 1 2108 CG2 VAL 303 1.703 45.122 1.000 14.80 6.041 ANISOU 2108 CG2 VAL 303 1876 1676 2069 -592 -639 3 2 2 2109 C VAL 303 3.467 9.328 46.303 1.000 13.88 ANISOU 2109 C VAL 303 870 1791 2613 75 -286 -375 2110 0 VAL 303 4.526 9.417 45.681 1.000 19.70 ANISOU 2110 O VAL 303 1064 2307 4114 -61 323 -304 3.271 10.046 47.393 1.000 13.77 323 - 999 2111 N MOTA ASN ANISOU 2111 N ASN 304 1681 1815 1737 -479 -388 1 4 0 2112 CA ASN 304 4.205 11.077 47.828 1.000 13.37 ATOM ASN ANISOU 2112 CA 304 1626 1240 2212 -213 -533 2 7 9 2113 СВ ASN ATOM 304 3.460 12.223 48.566 1.000 13.24 ANISOU 2113 CB ASN -243 -344 2 9 6 2114 CG MOTA ASN ANISOU 2114 CG ASN 304 1142 2326 1910 146 -88 230 ATOM 2115 OD1 ASN 304 2.776 13.283 46.540 1.000 16.65 ANISOU 2115 OD1 ASN 304 1408 2456 2464 107 185 9 304 1.263 13.126 48.209 1.000 17.45 304 1414 2961 2257 545 181 3 304 5.325 10.588 48.728 1.000 11.18 185 9 1 6 2116 ND2 ASN ANISOU 2116 ND2 ASN 181 3 1 5 2117 C ASN 10.588 48.728 1.000 11.18 ANISOU 2117 C 304 1382 ASN 1299 1566 -183 -163 1 1 2 MOTA 2118 0 304 6.396 ASN 11.232 48.699 1.000 12.07 ANISOU 2118 O 304 1325 ASN 1382 1879 -167 -66 -59 MOTA 2119 N ILE 305 5.092 9.541 49.516 1.000 12.56 ANISOU 2119 N 305-1791 ILE 1296 1685 -152 -232 2 0 2 2120 CA ATOM ILE 305 6.063 9.011 50.463 1.000 14.01 ANISOU 2120 CA ILE 305 2314 1393 1614 -55 -479 7 9 2121 CB ILE 305 5.781 9.493 51.906 1.000 14.44 ANISOU 2121 CB ILE 305 2223 1604 1659 -29 -217 1 5 7 2122 CG2 ILE 305 5.725 11.017 51.956 1.000 15.31 ANISOU 2122 CG2 ILE 305 1768 1608 2441 43 - 479 - 314 2123 CG1 ILE 305 4.543 8.853 52.498 1.000 14.83 ANISOU 2123 CG1 ILE 305 1779 1694 2163 27 - 307 - 153 ATOM 2124 CD1 ILE 305 4.163 9.252 53.900 1.000 28.68 ANISOU 2124 CD1 ILE 305 3788 5324 1786 -1491 381 9 2 ATOM 2125 C ANISOU 2125 C 305 6.059 7.487 ILE 50.389 1.000 12.79 ILE 305 1703 1355 1800 -260 -586 2 3 1 2126 O ATOM ILE 305 5.111 6.864 49.897 1.000 15.63 ANISOU 2126 O 305 1779 1564 306 7.170 6.896 ILE 2597 -185 -1008 277 2127 N ATOM ARG 306 7.170 6.896 306 1618 1389 306 7.340 5.435 306 1352 1366 306 8.111 4.965 306 1976 1941 306 8.203 3.472 306 2566 1953 306 2566 1953 306 2921 2361 306 7.078 3.198 306 2693 2844 306 6.948 3.186 50.829 1.000 13.04 ANISOU 2127 N ARG 1946 -368 -598 3 8 3 2128 CA ARG MOTA 50.868 1.000 11.82 ANISOU 2128 CA ARG 1773 -375 -154 4 4 4 2129 CB MOTA ARG 49.640 1.000 15.28 ANISOU 2129 CB ARG 1886 -368 -19 111 2130 CG ARG 49.395 1.000 17.16 ANISOU 2130 CG ARG -68 7 6 2001 -68 2131 CD ATOM ARG 47.937 1.000 19.51 ANISOU 2131 CD ARG 2130 -397 -396 - 302 ATOM 2132 NE 2.198 2844 3.10 ARG 47.212 1.000 20.65 ANISOU 2132 NE ARG 2309 -1056 -310 2 1 4 306 6.948 306 2006 2133 CZ ATOM ARG 45.893 1.000 17.11 ANISOU 2133 CZ ARG 2225 2268 45 - 91 5 9 6 MOTA 2134 NH1 ARG 306 8.013 3.065 45.083 1.000 21.58 ANISOU 2134 NH1 ARG 306 2405 2677 3116 -232 381 -669 306 5.734 306 2235 2135 NH2 ARG ATOM 3.301 45.365 1.000 17.51 ANISOU 2135 NH2 ARG 1550 2868 150 -484 - 162

- 160 -

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2136 C
                        ARG
                                  306 8.035
                                                      5.027
                                                                  52.155 1.000 13.45
ANISOU 2136 C
                                  306 2254
                        ARG
                                                      1018
                                                                 1837
                                                                              -246
                                                                                       -481 9 8
           2137 0
                       ARG
                                  306 9.006
                                                     5.682
                                                                  52.556 1.000 12.15
ANISOU 2137 O
                          ARG
                                  306 1902
                                                    1099
                                                                 1615
                                                                              -18
                                                                                        -362 - 80
           2138 N
                                  307 7.571
                                                  3.968
1620
ATOM
                          ARG
                                                                  52.811 1.000 18.19
ANISOU 2138 N
                          ARG
                                  307 3073
                                                                  2218
                                                                              -734
                                                                                       -938 7 9 2
                                 307 8.197 3.380
307 3053 1963
           2139 CA
MOTA
                          ARG
                                                                 53.989 1.000 19.20
ANISOU 2139 CA ARG
                                                                  2277
                                                                              -675
                                                                                       -1236 643
         2140 C
MOTA
                                  307 9.086 2.191
                          ARG
                                                                 53.611 1.000 23.08
                          ARG 307 4018 1905 2847 -270 -1885
ARG 307 8.636 1.292 52.895 1.000 35.93
ARG 307 6003 2403 5244 38 -3227 - 75
ANISOU 2140 C
                                                                                       -1885 3 2 9
         2141 0
ATOM
ANISOU 2141 O
                                                                              38 - 3227 - 791
                        ARG 307 7.131 2.918 54.997 1.000 28.25
ARG 307 5557 3297 1882 -1503 -277 5
           2142 CB
ATOM
ANISOU 2142 CB
                                                                              -1503 -277 5 0 9
                         ARG 307 6.032 3.921 55.275 1.000 33.39
MOTA
           2143 CG
ANISOU 2143 CG
                          ARG 307 4564 4859
                                                                 3261
                                                                             -1613 731
           2144 CD
                          ARG 307 5.022 3.523 56.317 1.000 40.42
ARG 307 6335 5701 3322 -1900 1263 9
ANISOU 2144 CD
                                                                             -1900 1263 9 7 1
           2145 NE

    307 5.605
    2.952
    57.529
    1.000 50.83

    307 8119
    7287
    3908
    -2786 105 1624

MOTA
                          ARG
ANISOU 2145 NE
                          ARG

      307
      8119
      7287
      3908
      -2786
      105
      1624

      307
      4.894
      2.441
      58.530
      1.000
      51.36

      307
      7424
      8064
      4025
      -3650
      -9662451

      307
      3.567
      2.422
      58.485
      1.000
      69.51

      307
      7586
      10951
      7874
      -6970
      -2008
      3245

      307
      5.489
      1.937
      59.600
      1.000
      59.99

      307
      10714
      8150
      3930
      -5986
      -3291
      2028

      308
      10.347
      2.147
      54.048
      1.000
      22.92

      308
      2759
      2587
      3364
      -589
      -200
      170

      308
      11.215
      1.009
      53.794
      1.000
      24.47

      308
      3382
      2649
      3268
      -360
      52150

      308
      10.602
      -0.252
      54.382
      1.000
      31.10

      308
      5251
      2520
      4044
      -768
      16279

ATOM
           2146 CZ
                          ARG
ANISOU 2146 CZ
                          ARG
           2147 NH1 ARG
ATOM
ANISOU 2147 NH1 ARG
           2148 NH2 ARG
ATOM
ANISOU 2148 NH2 ARG
ATOM
           2149 N
                          THR
ANISOU 2149 N
                          THR
           2150 CA
                          THR
ANISOU 2150 CA THR
ATOM
           2151 C
                          THR
                                 308 5251 2520 4044 -768 16 2 7 9
308 10.610 -1.292 53.718 1.000 31.44
ANISOU 2151 C
                          THR
                                                                             -768 16279
ATOM
           2152 0
                          THR
                        THR 308 4573 2676 4696 -457 -1745 THR 308 12.615 1.279 54.378 1.000 23.51
ANISOU 2152 O
                                                                             -457 -1745 -40
ATOM
           2153 CB
ANISOU 2153 CB
                         THR 308 3718 2086 3131
                                                                             413
                                                                                       -694 5 4 2
                                 308 13.195 2.410 53.705 1.000 23.61
           2154 OG1 THR
ATOM
ANISOU 2154 OG1 THR 308 2711 2503 3754
                                                                             153
                                                                                        437 - 9
MOTA
           2155 CG2 THR 308 13.573 0.141 54.117 1.000 26.37
ANISOU 2155 CG2 THR 308 4427 2796 2796
                                                                             927 -329 - 18
MOTA
           2156 N
                          SER 309 10.066 -0.156 55.596 1.000 28.39
ANISOU 2156 N SER 309 3759 2774 4252 -19 2 130

ATOM 2157 CA SER 309 9.488 -1.335 56.238 1.000 34.69

ANISOU 2157 CA SER 309 6110 3146 3925 -1066 -1089 1

ATOM 2158 C SER 309 8.109 -1.737 55.724 1.000 41.41
                                                                             -19 2 1300
                                                                             -1066 -1089 1626
                          SER 309 6442 3910 5383 -2171 -1170 2
SER 309 7.672 -2.884 55.952 1.000 57.05
SER 309 11389 5141 5146 -4907 -2077 2
SER 309 9.450 -1.104 57.755 1.000 31.61
SER 309 4863 2958 4188 -483 368 96
SER 309 8.485 -0.135 58.107 1.000 38.99
SER 309 4731 3477 6604 313 2248
ANISOU 2158 C
                                                                             -2171 -1170 2144
ATOM
           2159 O
ANISOU 2159 O
                                                                              -4907 -2077 2027
ATOM
           2160 CB
ANISOU 2160 CB
                                                                              -483 368 962
MOTA
           2161 OG
ANISOU 2161 OG
                          SER
                                 309 4731 3477
                                                                 6604
                                                                              313
                                                                                       -2249 - 496
           2162 N
MOTA
                                  310 7.391 -0.868 55.032 1.000 47.69
310 5502 5577 7040 -539 -1369 1
                          LYS
ANISOU 2162 N
                          LYS
                                                                              -539 -1369 1583
ATOM
           2163 FE
                                  312 8.574 13.466 54.055 1.000 11.05
                          IUM
ANISOU 2163 FE
                          IUM
                                  312 1690
                                                                 1351
                                                    1156
                                                                              -101 -237 7 1
ATOM
           2164 C1
                                  313 5.987 14.815 54.612 1.000 19.65
                          AKG
ANISOU 2164 C1
                          AKG
                                  313 2777
                                                    2119
                                                                  2572
                                                                              258
                                                                                       -117 5 5 6
           2165 01
ATOM
                          AKG
                                  313 4.799 15.240 54.659 1.000 20.82
ANISOU 2165 01
                          AKG
                                  313 2957
                                                   2293
                                                                  2659 514 -234 2 6 4
ATOM
           2166 02
                                 313 6.643
                          AKG
                                                   14.144 53.787 1.000 17.79
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- 161 -ANISOU 2166 O2 AKG 313 2407 1765 2587 74 - 377 429 2167 C2 MOTA AKG 313 6.867 15.178 55.844 1.000 20.08 ANISOU 2167 C2 AKG 313 1997 2566 3068 -528 419 -3 14.661 55.821 1.000 17.60 2566 -528 419 -399 2168 05 ATOM AKG 313 7.982 313 2289 2066 2334 -314 226 -3 313 6.272 16.080 56.872 1.000 21.69 ANISOU 2168 05 AKG -314 226 -252 2169 C3 ATOM AKG ANISOU 2169 C3 AKG 1910 313 2751 3581 240 62 - 327 313 7.318 16.741 57.716 1.000 21.50 ATOM 2170 C4 AKG ANISOU 2170 C4 AKG 313 3246 1761 3160 199 -143 - 185 ATOM 2171 C5 313 6.923 17.816 58.672 1.000 22.58 AKG ANISOU 2171 C5 AKG 313 3122 1840 3618 755 -495 - 313 ATOM 2172 03 AKG 313 7.754 18.591 59.124 1.000 27.48 AKG 313 7.754 18.591 59.124 1.000 27.48
AKG 313 3581 2470 4389 -34 602 AKG 313 5.660 17.889 58.999 1.000 28.55
AKG 313 3191 2809 4846 612 -246 SO4 401 11.676 0.439 24.942 1.000 40.14
SO4 401 11.293 0.826 26.321 1.000 33.12
SO4 401 12.501 -0.829 25.014 1.000 35.79
SO4 401 10.430 0.189 24.129 1.000 54.89 ANISOU 2172 03 -34 602 -1266 ATOM 2173 O4 ANISOU 2173 O4 612 -246 -1148 2174 S ATOM MOTA 2175 01 2176 02 ATOM 2177 03 MOTA

 401
 12.500
 1.520
 24.329
 1.000
 44.80

 501
 -6.455
 10.219
 44.319
 1.000
 14.29

 502
 -10.520
 18.612
 50.560
 1.000
 12.86

 503
 -8.644
 16.907
 47.858
 1.000
 16.83

 504
 -10.313
 20.800
 43.074
 1.000
 16.10

 505
 -6.051
 19.199
 52.602
 1.000
 16.38

 506
 -6.873
 24.642
 47.100
 1.000
 20.55

 507
 10.676
 -4.179
 46.406
 1.000
 27.41

 508
 -0.077
 21.786
 40.872
 1.000
 15.22

 509
 5.761
 13.656
 46.041
 1.000
 17.40

 510
 29.135
 31.449
 51.982
 1.000
 18.40

 511
 26.032
 32.724
 52.741
 1.000
 17.03

 512
 10.965
 32.371
 46.000
 1.000
 16.70

 513
 23.871
 24.457
 58.649
 1.000
 18.71 401 12.500 1.520 24.329 1.000 44.80 ATOM 2178 04 SO4 2179 OW MOTA нон 2180 OW MOTA HOH MOTA 2181 OW нон MOTA 2182 OW HOH ATOM 2183 OW HOH MOTA 2184 OW HOH ATOM 2185 OW HOH ATOM 2186 OW нон ATOM 2187 OW HOH ATOM 2188 OW HOH ATOM 2189 OW HOH MOTA 2190 OW HOH ATOM 2191 OW HOH 2192 OW MOTA HOH MOTA 2193 OW HOH ATOM 2194 OW HOH 516 21.429 11.721 55.329 1.000 18.39 2195 OW MOTA HOH 517 9.122 15.567 53.585 1.000 24.87 2196 OW ATOM HOH 518 27.843 17.352 53.437 1.000 27.76 ATOM 2197 OW 519 -14.415 20.029 44.444 1.000 23.47 HOHMOTA 2198 OW HOH 520 15.253 33.050 51.771 1.000 27.20 MOTA 2199 OW HOH 521 14.080 31.486 44.302 1.000 21.58 MOTA 2200 OW HOH 522 17.770 33.842 53.596 1.000 23.56 2201 OW ATOM 523 3.671 24.673 36.173 1.000 20.95 HOH524 -15.683 28.618 52.535 1.000 24.05 525 -5.386 20.413 39.013 1.000 26.85 MOTA 2202 OW нон MOTA 2203 OW нон 2204 OW ATOM HOH 526 10.417 27.949 58.778 1.000 28.33 ATOM 2205 OW HOH 527 23.165 19.592 62.202 1.000 29.36 528 23.736 10.550 55.737 1.000 24.02 529 -1.662 28.650 42.485 1.000 21.62 530 -4.689 10.177 46.511 1.000 31.65 ATOM 2206 OW HOH ATOM 2207 OW HOHATOM 2208 OW HOH ATOM 2209 OW 531 1.545 35.657 50.866 1.000 19.59 532 0.980 22.687 36.818 1.000 30.57 HOHATOM 2210 OW HOH 533 -12.450 16.848 56.071 1.000 28.42 534 -9.418 16.139 51.364 1.000 22.60 535 32.711 25.816 43.116 1.000 31.44 536 27.068 24.587 55.468 1.000 23.32 537 13.523 11.832 51.199 1.000 10.73 ATOM 2211 OW HOH ATOM 2212 OW HOH ATOM 2213 OW HOH ATOM 2214 OW HOH 2215 OW ATOM HOH 2216 OW ATOM 538 8.513 539 0.922 HOH 16.158 35.074 1.000 12.26 539 0.922 2.590 35.058 1.000 14.79 540 -1.548 3.709 34.484 1.000 14.25 541 11.711 16.898 30.416 1.000 17.84 ATOM 2217 OW HOH MOTA 2218 OW HOH ATOM 2219 OW HOH

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ATOM
       2220 OW
                     542 15.389
                                 11.536 32.065 1.000 17.88
                HOH
       2221 OW
                     543 18.496
                                6.995
MOTA
                HOH
                                         52.191 1.000 17.47
ATOM
       2222 OW
                     544 19.848
                                22.580
                                        35.334 1.000 17.28
                HOH
MOTA
       2223 OW
                нон
                     545 -0.387 4.787
                                         41.967 1.000 13.22
MOTA
       2224 OW
                HOH
                     546 23.502 12.662
                                        35.308 1.000 18.14
                     547 10.332
       2225 OW
ATOM
                HOH
                                25.236
                                        33.926 1.000 19.05
       2226 OW
                     548 21.447 20.605 34.090 1.000 17.24
ATOM
                HOH
       2227 OW
                нон
                     549 8.164
                                         27.077 1.000 25.40
MOTA
                                 7.685
ATOM
       2228 OW
                HOH
                     550 14.393 -5.127
                                        40.321 1.000 15.88
       2229 OW
MOTA
                HOH
                     551 12.873 29.356 39.662 1.000 16.45
       2230 OW
ATOM
                HOH
                     552 11.974 24.144 58.426 1.000 19.71
       2231 OW
                     553 17.521 7.949
                                         33.182 1.000 17.90
ATOM
                HOH
       2232 OW
ATOM
                HOH
                     554 3.401
                                 2.691
                                         43.340 1.000 23.76
       2233 OW
                     555 18.669 28.057 40.079 1.000 18.44
MOTA
                HOH
       2234 OW
                     556 10.827 12.928 30.017 1.000 19.57
                HOH
ATOM
       2235 OW
                HOH
                    557 20.630 16.270 66.466 1.000 20.84
ATOM
ATOM
       2236 OW
                HOH
                    558 11.315 20.266 64.044 1.000 21.62
       2237 OW
ATOM
                HOH
                     559 26.277 14.516 43.946 1.000 16.22
       2238 OW
                нон
                     560 9.616
                                 15.488 32.365 1.000 19.40
ATOM
ATOM
       2239 OW
                HOH
                     561 8.888
                                 4.903
                                         27.857 1.000 22.74
                     562 20.496 -1.851 42.511 1.000 22.98
563 17.033 29.415 38.332 1.000 26.36
ATOM
       2240 OW
                HOH
       2241 OW
MOTA
                HOH
                     564 18.595
                                         37.697
       2242
                                 6.141
                                                1.000 25.10
MOTA
            OW
                HOH
       2243
                     565 22.446 13.893
                                        31.420 1.000 29.00
ATOM
            OW
                HOH
                                 3.577
                                         28.350 1.000 27.82
MOTA
       2244 OW
                HOH
                     566 6.586
       2245 OW
                     567 6.250
                                 20.077
                                        30.961 1.000 23.27
MOTA
                НОН
       2246 OW
ATOM
                     568 7.341
                                 16.113
                                        31.186 1.000 28.59
                HOH
ATOM
       2247 OW
                нон
                     569 16.090 32.070
                                        42.552
                                                1.000 33.08
MOTA
       2248 OW
                HOH
                     570 11.500
                                 28.806
                                        37.258 1.000 25.17
                     571 12.901
       2249 OW
                HOH
                                        58.591 1.000 28.58
ATOM
                                 26.768
ATOM
       2250 OW
                HOH
                     572 -17.071 17.043 50.450 1.000 28.82
ATOM
       2251 OW
                HOH
                     573 25.262
                                 7.705
                                         37.199 1.000 3.9.05
ATOM
       2252 OW
                HOH
                     574 32.884
                                 26.440 51.734 1.000 29.03
       2253 OW
                                 19.088 42.527 1.000 14.86
ATOM
                HOH
                     575 -1.199
       2254 OW
                                 33.026 63.392 1.000 29.56
ATOM
                HOH
                     576 -4.389
ATOM
       2255 OW
                HOH
                     577 17.569 25.732
                                         32.249 1.000 20.62
MOTA
       2256 OW
                HOH
                     578 -19.107 12.822 67.516 1.000 22.35
ATOM
       2257 OW
                HOH
                     579 29.333 19.198 51.975 1.000 22.51
MOTA
       2258 OW
                HOH
                     580 27.950 27.635 51.903 1.000 25.40
MOTA
       2259 OW
                                         68.535 1.000 21.19
                НОН
                     581 -21.085 14.501
                                         33.953 1.000 25.29
66.894 1.000 33.92
                     582 1.529
ATOM
       2260 OW
                HOH
                                 17.378
ATOM
       2261 OW
                HOH
                     583 9.138
                                 20.887
                                         44.780 1.000 17.48
43.347 1.000 22.09
29.046 1.000 20.79
       2262 OW
MOTA
                HOH
                      584 -11.896 19.091
ATOM
       2263 OW
                HOH
                      585 6.382
                                 12.597
ATOM
       2264 OW
                HOH
                      586 17.762
                                 21.268
                                         41.729 1.000 29.68
ATOM
       2265 OW
                HOH
                      587 -11.500 25.438
                                         29.689 1.000 27.70
                      588 7.877
       2266 OW
ATOM
                HOH
                                 1.046
                      589 27.985
                                         42.235 1.000 25.91
ATOM
       2267 OW
                                 13.540
                HOH
                                         34.021 1.000 20.41
MOTA
       2268 OW
                      590 1.276
                HOH
                                  14.852
                                         41.242 1.000 26.77
MOTA
       2269 OW
                      591 24.622
                                 24.179
                HOH
                                         36.006 1.000 27.92
ATOM
       2270 OW
                                  14.096
                HOH
                      592 0.404
       2271 OW
                                 36.981 57.827 1.000 31.86
MOTA
                HOH
                      593 -2.835
ATOM
       2272 OW
                 HOH
                      594 3.276
                                  0.788
                                         39.940 1.000 32.07
ATOM
       2273 OW
                 HOH
                      595 11.025 -8.794 31.468 1.000 27.18
                                  2.276
ATOM
       2274 OW
                      596 6.301
                                         42.639 1.000 29.74
                 HOH
        2275 OW
                      597 29.302
                                  16.146 62.924 1.000 43.75
ATOM
                 HOH
        2276 OW
MOTA
                 HOH
                      598 19.039
                                  20.964 67.011 1.000 30.85
        2277 OW
                                  22.088 64.518 1.000 42.62
MOTA
                 HOH
                      599 8.380
        2278 OW
                                         34.742 1.000 25.74
ATOM
                 HOH
                     600 21.480 10.826
        2279 OW
ATOM
                 HOH 601 -2.907
                                  21.956 38.566 1.000 30.92
ATOM
        2280 OW
                 HOH
                     602 -3.928 29.841 43.352 1.000 43.96
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- 163 -MOTA 2281 OW нон 603 2.885 21.563 34.437 1.000 33.10 MOTA 2282 OW 604 11.801 HOH 6.043 25.270 1.000 38.18 ATOM 2283 OW HOH 605 -1.019 17.197 40.472 1.000 18.48 MOTA 2284 OW HOH 606 18.382 23.349 68.110 1.000 22.54 2285 OW ATOM HOH 607 -8.141 8.137 45.609 1.000 17.64 51.700 1.000 24.29 2286 OW ATOM HOH 608 5.022 2.667 2287 OW ATOM HOH 609 17.557 10.755 33.490 1.000 21.94 2288 OW MOTA HOH 610 11.222 49.675 1.000 20.61 50.509 1.000 22.18 1.201 2289 OW ATOM HOH 611 4.243 35.047 56.082 1.000 22.08 36.791 1.000 32.32 52.739 1.000 31.83 30.674 1.000 24.77 31.445 1.000 25.97 2290 OW ATOM 612 11.103 HOH 4.031 2291 OW MOTA 613 11.366 HOH 31.522 2292 OW ATOM HOH 614 -21.189 24.787 ATOM 2293 OW нон 615 7.847 -1.491 2294 OW ATOM HOH 616 19.041 11.937 2295 OW ATOM HOH 617 6.221 29.879 40.410 1.000 29.24 2296 OW ATOM нон 618 17.266 5.933 35.280 1.000 23.72 ATOM 2297 OW HOH 619 5.983 -7.215 28.510 1.000 28.19 ATOM 2298 OW HOH 620 22.574 8.129 57.639 1.000 30.97 ATOM 2299 OW HOH 621 2.553 60.287 1.000 28.77 7.806 ATOM 2300 OW HOH 622 29.939 25.812 51.234 1.000 34.00 ATOM 2301 OW нон 623 2.205 53.632 1.000 25.88 34.823 ATOM 2302 OW HOH 624 18.091 13.838 67.343 1.000 28.46 2303 OW ATOM HOH 625 8.342 58.475 1.000 26.84 3.195 2304 OW MOTA НОН 626 -16.086 18.427 42.790 1.000 31.11 MOTA 2305 OW HOH 627 -2.098 13.445 35.620 1.000 27.48 ATOM 2306 OW HOH 628 0.481 30.471 42.834 1.000 32.55 2307 OW ATOM НОН 629 13.368 33.845 42.899 1.000 28.70 2308 OW ATOM 630 -13.792 14.642 51.533 1.000 25.58 631 3.299 1.461 29.242 1.000 39.62 HOH ATOM 2309 OW HOH 29.242 1.000 39.62 2310 OW MOTA нон 632 -16.012 20.690 46.705 1.000 27.75 2311 OW ATOM 633 19.606 8.142 нон 31.259 1.000 27.02 2312 OW ATOM 634 5.077 7.954 635 -1.502 6.963 HOH 57.205 1.000 30.59 ATOM 2313 OW HOH 45.877 1.000 35.68 ATOM 2314 OW HOH 636 9.974 17.449 38.804 1.000 21.84 637 -22.829 12.836 67.228 1.000 25.04 638 6.275 34.333 39.722 1.000 25.88 639 2.248 19.798 56.051 1.000 26.67 ATOM 2315 OW HOH ATOM 2316 OW HOH ATOM 2317 OW нон ATOM 2318 OW 67.454 1.000 31.34 28.911 1.000 29.96 60.074 1.000 28.13 нон 640 -20.552 17.013 ATOM 2319 OW НОН 641 9.298 16.570 ATOM 2320 OW HOH 642 -1.732 11.113 ATOM 2321 OW HOH 44.657 1.000 36.36 33.576 1.000 34.90 31.570 1.000 32.66 29.009 1.000 34.61 643 34.157 23.604 ATOM 2322 OW 644 24.298 HOH 20.199 ATOM 2323 OW HOH 645 13.803 -4.667 MOTA 2324 OW HOH 646 6.295 -2.594 ATOM 2325 OW 49.318 1.000 28.08 46.868 1.000 38.32 HOH 647 5.623 37.039 MOTA 2326 OW нон 648 -18.805 19.286 ATOM 2327 OW НОН 649 16.026 35.829 1.000 34.45 49.382 2328 OW ATOM нон 650 -12.187 28.769 45.330 1.000 27.36 55.101 1.000 27.43 ATOM 2329 OW нон 651 21.344 5.778 MOTA 2330 OW нон 652 -1.848 2.125 32.240 1.000 32.02 ATOM 2331 OW HOH 653 -14.568 18.811 55.775 1.000 29.95 ATOM 2332 OW HOH 654 -8.655 26.254 38.301 1.000 32.07 ATOM 2333 OW HOH 655 18.836 13.542 28.102 1.000 32.24 ATOM 2334 OW НОН 656 16.217 14.669 25.619 1.000 33.35 ATOM 2335 OW нон 657 28.678 14.477 38.043 1.000 30.94 ATOM 2336 OW нон 658 -11.834 15.408 1.000 33.25 53.330 ATOM 2337 OW НОН 659 -1.317 38.273 59.599 1.000 34.45 ATOM 2338 OW HOH 660 8.784 13.918 28.681 1.000 33.62 ATOM 2339 OW HOH661 -3.058 14.508 47.405 1.000 28.79 ATOM 2340 OW HOH 662 10.968 33.651 38.533 1.000 36.21 ATOM 2341 OW HOH 663 28.960 21.602 53.665 1.000 29.25

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ATOM	2342	OW	нон	664	-10.709	26 000	20 17=	1 000 10 71
ATOM	2343	OW	HOH	665	17.790		39.175	1.000 42.71
ATOM	2344	OW	HOH	666		7.093	55.023	1.000 30.29
ATOM	2345				6.404	24.865	29.848	1.000 34.55
		OW	нон	667	-15.418	19.777	58.341	1.000 33.82
ATOM	2346	OW	нон	668	0.000	0.000	37.259	0.330 49.90
ATOM	2347	WO	нон	669	19.652	24.610	33.660	1.000 31.77
ATOM	2348	WO	нон	670	17.188	9.619	29.950	1.000 29.94
ATOM	2349	OM	нон	671	17.708	2.958	28.338	1.000 34.94
ATOM	2350	OM	нон	672	-0.059	3.652	30.079	1.000 32.23
\mathtt{ATOM}	2351	ow	HOH	673	29.037	20.923	56.153	1.000 28.52
ATOM	2352	ow	HOH	67 <u>4</u>	-15.435	31.088	53.795	1.000 35.61
ATOM	2353	ow	HOH	675	-12.846	21.220	61.856	1.000 38.79
ATOM	2354	WO	HOH	676	10.299	39.666	49.554	1.000 40.30
ATOM	2355	OW	HOH	677	-5.921	28.822	41.521	1.000 34.01
ATOM	2356	OW	нон	678	6.029	39.991	46.094	1.000 42.69
ATOM	2357	OW	HOH	679	35.052	23.156	52.356	1.000 40.17
ATOM	2358	OW	нон	680	-12.008	38.355	51.601	1.000 35.18
ATOM	2359	OW	нон	681	3.061	13.047	53.152	1.000 35.17
ATOM	2360	OW	нон	682	1.379	2.075	27.532	1.000 46.38
ATOM	2361	OW	нон	683	-0.516	-2.480	37.686	1.000 21.77
ATOM	2362	OW	нон	684	4.567	10.310	43.503	1.000 24 . 86
ATOM	2363	OW	нон	685	19.443	5.558	61.133	1.000 24.30
ATOM	2364	OW	нон	686	3.205	29.499	40.656	1.000 36.00
ATOM	2365	OW	нон	687	32.498	16.774	43.447	1.000 3 6 . 3 9
ATOM	2366	OW	нон	688	28.166	23.113	57.593	1.000 41.16
ATOM	2367	OW	нон	689	-17.023	23.220	46.759	1.000 3 3 . 3 6
ATOM	2368	OW	HOH	690	15.567			
ATOM	2369	OW	нон		15.367 11.780	7.782	28.910	1.000 32.51
MOTA	2370	OW	нон			30.287	57.203	1.000 33.34
ATOM	2371	OW		692	24.449	12.699	32.400	1.000 34.99
AION	1 / د ت	$\mathcal{O}_{\mathcal{M}}$	нон	693	26.200	25.005	57.918	1.000 39.38

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CLAIMS

- Deacetoxycephalosporin C synthase (DAOCS) having a structure designated by the X-ray co-ordinates of structure A or structure B herein.
- 2. DAOCS in the form of a complex with a metal, e.g. iron or lead, and optionally in the presence of a substrate and/or a substrate analogue or inhibitor, having a structure designated by the X-ray co-ordinates herein.
- 3. DAOCS as claimed in claim 2, wherein the substrate is penicillin N, penicillin G, 2-oxoglutarate or dioxygen, and the inhibitor is selected from N-oxalylamino acids, pyridine-carboxylates and nitrous oxide.
- 4. Use of the three-dimensional structure of DAOCS for the modification of DAOCS or other related 2-oxoglutarate dependent enzyme.
 - 5. Use as claimed in claim 4, wherein the related 2-oxoglutarate dependent enzyme is DACS, DAOC/DACS or the oxygenase enzyme involved in the introduction of the 7α -methoxy group into cephamycin C.
 - 6. Use as claimed in claim 5 for the modification of DAOCS, DACS or DAOC/DACS such that they accept unnatural substrates more efficiently than the wild type enzymes.

7. Use as claimed in claim 5 for the modification of DAOCS, DACS, DAOC/DACS such that they convert natural substrates to pharmaceuticals or useful intermediates in the preparation of pharmaceuticals.

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8. Use as claimed in claim 6 wherein the unnatural substrates are penicillins including penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, or penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain.

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- 9. Use as claimed in claim 6 wherein the unnatural substrate is a cephalosporin.
- 10. Use as claimed in claim 6 wherein the unnatural substrate is an amino acid, including the proteinogenic amino acids, or a peptide.
 - 11. Use as claimed in any one of claims 6-8, wherein penicillin G, penicillin V, another unnatural substrate or penicillin N is converted to a cephalosporin or exomethylene cephalosporin.

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- An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at
- Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

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- 14. An enzyme according to claim 12 or claim 13 which is a mutant of DAOCS or DACS or DAOC/DACS.
- 15. An enzyme as claimed in any one of claims 12-14, wherein both the side chain and the penicillin/cephalosporin binding sites of penicillin N or DAOC are modified and at least one of the residues specified in claims 12 and 13 is changed or deleted.
- 16. An enzyme as claimed in any one of claims 12-15, wherein
 two or more complementary mutations are introduced to create or delete a
 binding interaction, including H-bonds, electrostatic, or hydrophobic
 interactions.
 - 17. A gene encoding for the enzyme of any one of claims 12-16.

- 18. A micro-organism capable of expressing the gene of claim 17 under fermentation conditions.
- 19. Use of micro-organisms of claim 18 for the production of
 30 beta-lactams of the penicillin or cephalosporin (including cepham) families.

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- 20. Use as claimed in claim 19 wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway including isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 21. A method which comprises using the three-dimensional structure of DAOCS for determining or predicting the structure of another related 2-oxoglutarate dependent enzyme or related enzyme not from the penicillin and cephalosporin biosynthesis pathway, and using the structural information so obtained for modifying the other enzyme or for designing an inhibitor for the other enzyme.
- A method as claimed in claim 21 wherein the said other
 related 2-oxoglutarate dependent enzyme or related enzyme is
 1-aminocylopropane-1-carboxylate oxidase, gibberellin C-20 oxidase,
 flavone synthase, flavanone 3β-hydroxylase, hyoscyamine 6β-hydroxylase,
 prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, lysyl
 hydroxylase, proline hydroxylases, γ-butyrobetaine hydroxylase, enzymes
 in herbicide resistance mechanisms, clavaminate synthase, an oxygenase
 enzyme involved in the biosynthesis of carbapenems, the so called
 ethylene forming enzyme from *Pseudomonas syringe*,
 p-hydroxyphenylpyruvate dioxygenase, and an oxygenase enzyme
 involved in the oxidation of phytol in human liver peroxisomes.

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A method as claimed in claim 21 or 22, wherein the said other enzyme is modified, by deletion or addition or alteration; at one or more of the sites defined in claim 12 or claim 13; or using the following information for the design or an inhibitor: Asp185, His183 and His243 act as ligands to the iron; Arg258 and Ser260 and the Fe bind the

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2-oxoglutarate; Met180, Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33, Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are important for the construction of the part of the active site binding 2-oxoglutarate; and Arg160 and Arg162 are important for binding an amino acid or peptide derived substrate.

- A method as claimed in any one of claims 21-23, wherein the said other enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the treatment of human diseases including fibrotic diseases including liver cirrhosis and arthritis.
- A method as claimed in any one of claims 21-23, wherein the said other enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.
- A method as claimed in any one of claims 21-23, wherein the said other enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.

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Fig.2.

Tyr-302

Arg-256

Ser-260

$$H_1 = \text{His-183}$$
 $H_2 = \text{His-243}$

Fig.2.

 A_{Sp-304}
 A_{Sp-185}
 A_{Sp-304}
 A_{Sp-304}
 A_{Sp-304}
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 A_{Sp-305}
 A_{Sp-306}
 A_{Sp-306}
 A_{Sp-306}
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INTERNATIONAL SEARCH REPORT

Inte. .ional Application No PCT/GB 98/03860

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A" docum consid	ategories of cited documents: ent defining the general state of the art which is not dered to be of particular relevance document but published on or after the international	"T" later document published after the int or priority date and not in conflict with cited to understand the principle or the invention	n the application but neory underlying the				
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Name and	mailing address of the ISA European Patent Office, P.B. 5818 Patentiaan 2 NL - 2280 HV Rijswijk	Authorized officer					
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